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FISCAL YEAR 1985 DEPARTMENT OF ENERGY AUTHORIZATION

(Supporting Research and Technical Analysis)

HEARING

BEFORE THE

SUBCOMMITTEE ON
ENERGY DEVELOPMENT AND APPLICATIONS

OF THE

COMMITTEE ON
SCIENCE AND TECHNOLOGY
U.S. HOUSE OF REPRESENTATIVES

NINETY-EIGHTH CONGRESS

SECOND SESSION

FEBRUARY 23, 1984

[No. 131]

VOLUME VII-B

Printed for the use of the
Committee on Science and Technology

U.S. GOVERNMENT PRINTING OFFICE

40-574 O WASHINGTON : 1985

H701-47

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CONTENTS

WITNESSES

Page

Appendix I: Questions and answers submitted for the record—Continued
Dr. Alvin W. Trivelpiece—Continued
E. Chemical Sciences Subprogram 1
F. Nuclear Sciences Subprogram 218
1.0 Heavy Ion Fusion Accelerator Research (HIFAR)... 321
2.0 Isotopes Preparations 348
G. Applied Mathematical Sciences Subprogram 350
H. Engineering Research Program 442
I. Geosciences Research Program 532
J. Advanced Energy Projects (AEP) Subprogram 668
K. Biological Energy Research (BER) Subprogram 725
L. BES Program Direction 793
M. Construction 803
1.0 Project 84-ER-141, General Plant Projects 803
2.0 Project 85-ER-400, General Plant Projects 803
3.0 Project 84-ER-141, Accelerator Improvements and Modifications 804
4.0 Project 85-ER-401, Accelerator Improvements and Modifications 804
5.0 Project 85-ER-402, Stanford Synchrotron Radiation Laboratory Enhancement 804
6.0 Project 85-ER-403, Ion Collision Facility, Kansas State University 805
7.0 Project 84-ER-411, Beam Lines and Support Area Construction, NSLS 807
II. Energy Research Analysis 809
III. University Research Support (URS) 865
A. Holifield Tables 865
B. University-Laboratory Cooperative Program 868
C. University Reactor Fuel Assistance 870
D. Energy Manpower Assessment 875
E. Energy Education and Training 879
IV. University Research Instrumentation (URI) 882
V. Advisory and Oversight Program Direction 885
A. Holifield Tables 894
B. Laboratory Appraisal Process 895
C. ERAB Multiprogram Laboratory Panel September 1982 Report 897
1.0 Appropriate Roles and Mission of the Laboratories Vis-a-Vis Universities and Industry 897
2.0 Scientific and Technological Capabilities of the Laboratories 897
3.0 The Department's Policies and Procedures with Respect to the Laboratories 898
4.0 Effectiveness of the Department's Use of the Laboratories in Meeting Its Energy Objectives 899
5.0 Alternative Strategies for Making Best Use of the Laboratories in a Constrained Budgetary Environment 902
D. White House Science Council Federal Laboratory Review Panel May 1983 Report 903

Page

1.0 Mission 903
2.0 Resources: Personnel 903
3.0 Resources: Funding 904
4.0 Management 905
5.0 Interaction with Universities, Industry, and Users of Research Results 907
E. President's Private Sector Survey on Cost Control (PPSSCC) 908
VI. Multiprogram General Purpose Facilities (MGPF) 909
A. Holifield Tables 914
B. Projects 916
1.0 Project 85-R-701, Central Chilled Water Facility (BNL) 916
2.0 Project 85-R-702, Replace Laboratory Roofs (ANL) 917
3.0 Project 85-R-703, Electrical Distribution System Rest. (ORNL) 917
4.0 Project 85-R-704, Rehab. Underground Steam System (ANL) 918
5.0 Project 85-R-706, Medical Facility Replacement (LLNL) 918
6.0 Project 85-R-707, Replace Site Fire Alarm System (ANL) 925
7.0 Project 85-R-709, Est. Central Chilled Water Plant (ANL) 925
8.0 Project 85-R-711, Upgrade Environmental Monitoring (ORNL) 926
9.0 Project 85-R-712, Modify Central Chilled Water Plant (ORNL) 926
10.0 Project 84-ER-103, Road Repair (LBL, INEL, RL, ANL) 927
11.0 Project 84-ER-102, Cooling Water Facility Rest. (ORNL) 929
12.0 Project 85-ER-101, Rehab. Old Town Utilities (LBL) 930
13.0 Project 84-E-310, Utility Replacement and Upgrade (BNL) 930
14.0 Project 83-E-309, Electronics Facility (ANL) 931
15.0 Project 83-E-308, Rehab. Power Systems (INEL, LLNL, RL, ORNL) 932
16.0 Project 82-E-302, Security Facility (ANL) 934
VII. Energy Science Research Computation (ESRC) 935
Supporting Research and Technical Analysis, March 19, 1984 938
Professor George C. Pimentel 945
Dr. Albert Narath 950
Dr. Peter M. Eisenberger and Dr. Michael L. Knotek 956
Dr. Hermann A. Grunder and Dr. Gabor A. Somorjai 964
Dr. Robert H. Pry 989
Dr. Frederick Seitz 1000
Appendix II: Additional materials for the record:
"Report of the ad hoc Panel to Review the Lawrence Berkeley Laboratory Proposal for a National Center for Advanced Materials (NCAM)," August 31, 1983 1004
"Planning Study for Advanced National Synchrotron-Radiation Facilities," Printed March 14, 1984 1070
"Major Facilities for Materials Research and Related Disciplines," Major Materials Facilities Committee, Commission on Physical Sciences, Mathematics and Resources, National Research Council, National Academy Press, Washington, DC, 1984 1181
"Report of the NCAM Industry Participation Workshop," May 23, 1983, Lawrence Berkeley Laboratory, PUB-5101 1266
"Workshop on the Electronic Materials Program," October 10-12, 1983, Lawrence Berkeley Laboratory, February 1984, PUB-5110 1286
"Workshop on CAM Program on Polymers and Polymer Composites," October 24-25, 1983, Lawrence Berkeley Laboratory, October 1983, PUB-5107 1370

Page

"Workshop on CAM Program on Metal Compounds as Catalysts," October 27-28, 1983, Lawrence Berkeley Laboratory, October 1983, PUB-5106 1418
"Materials Research and Development," Prepared by the Materials Research and Development Panel, November 1983, A Report of the Energy Research Advisory Board to the U.S. Department of Energy, DOE/S-0027 1474
Statement submitted by the Association of American Universities 1507
Department of Energy fiscal year congressional budget request:
Energy Supply Research and Development, Volume 3 1533
Program Overview 1534
Basic Energy Sciences 1536
Energy Research Analysis 1600
University Research Support 1603
University Research Instrumentation 1610
Advisory and Oversight Program Direction 1612
Multiprogram General Purpose Facilities 1614

E. Chemical Sciences Subprogram

1. **What is the detailed budget structure of the Chemical Sciences subprogram? What types of work are funded by each of these budget categories?**

Answer: The Chemical Sciences budget is broken down into funds for operating expenses, capital equipment and construction. General plant projects (GPP) and Accelerator & Reactor Improvement and Modification Projects (ARIM) are included under construction, and general purpose equipment (GPE) under capital equipment. Operating expenses are divided between two budget categories Fundamental Interactions (01) and Processes and Techniques (02).

In the Fundamental Interactions category (01), basic research is supported in photochemical and radiation sciences, chemical physics, and atomic physics. In photochemical and radiation sciences, the photochemical studies are largely devoted to captures of visible light and its conversion to electricity or fuels. Research related to solar photochemical conversion encompasses photoelectrochemistry, homogeneous and heterogeneous redox systems, charge separation in natural photosynthetic systems and in artificial organized assemblies, and photochemistry and photophysics related to solar photoconversion. Radiation chemical studies are conducted on the chemical effects produced by absorption of ionizing radiation and hot atom chemical studies on reactions of highly energetic atoms recoiling from nuclear decay. In chemical physics, the research involves theoretical quantum mechanics, statistical mechanics, chemical dynamics, energy transfer, and molecular structure and spectroscopy. Scientists are investigating the rapid and complex chemical sequences which are fundamental to combustion, using advanced laser diagnostic methods, modeling, and theoretical and kinetic studies of elementary combustion reactions. Research in surface chemistry explores the mechanisms of adsorption, chemisorption and reactions of molecules on catalytic surfaces. The atomic physics program supports experimental and theoretical studies of atom and ion structures, energy levels and lifetimes of quantum states, and of transport and exchange processes involving energy, momentum and matter.

In Processes and Techniques (02), research is supported in chemical energy, separations science, analytical chemistry, and chemical engineering sciences. Chemical energy is rather broadbased, comprising, in the main, research in inorganic, organic and physical chemistry. The emphasis in the chemical energy research is on developing an understanding of the chemical principles underlying technologies related to energy production. These include heterogeneous catalysis, homogeneous catalysis and the chemistry of coal. The separations science and analytical chemistry efforts involve studies of the principles underlying chemical, physical and isotopic separations as well as the development of new analytical techniques. The activities in chemical engineering sciences are the more scientific and energy related aspects of chemical engineering, such as transport phenomena, thermodynamics, turbulent flow and rate processes.

A more complete picture of the research supported under these budget categories can be obtained from the annual booklet, Summaries of Research in the Chemical Sciences. The most recent one is for FY 83, DOE/ER-0144/1.

2. **For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.**

Answer: The funding by year for the Chemical Sciences subprogram is:

(Budget Authority In Millions)

	FY 81	FY 82	FY 83	FY 84	FY 85
Operating					
Fundamental Interactions (01)	35.84	40.26	43.50	46.75	50.66
Processes and Techniques (02)	23.50	24.24	26.50	28.75	30.27
Total Chemical Sciences	59.34	64.50	70.00	75.50	80.93
Equipment*	4.00	4.93	5.51	6.52	8.84[1]
Construction*	3.20	0	0.40	0.45	8.05[2]

1 Includes $2 M for GPE at ANL.
2 Includes $5.75 M for GPP, principally at ANL.

* Equipment and Construction funds are not apportioned by budget category below the subprogram level.

3. **For the period FY 1981 - FY 1985, please identify, by budget category and by facility, that portion of Chemical Sciences funding going for the support of facilities, such as the National Synchrotron Light Source, etc.**

Answer: Chemical Sciences funds facility operation and research at two major facilities: the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (in addition to funding of NSLS by Materials Sciences) and the Combustion Research Facility (CRF) at Sandia National Laboratories-Livermore (in addition to funding of research at CRF by other DOE programs). The Chemical Sciences funding at these two facilities is:

(Budget Authority In Thousands)

		FY 81	FY 82	FY 83	FY 84	FY 85
NSLS						
Facility Operations	(01)	500	2300	3800	4470	5600
Research						
	(01)	500	1300	1470	1530	1650
	(02)	0	0	100	350	380
CRF						
Facility Operations	(01)	1900	1930	2170	2490	2750
Research						
	(01)	1700	2320	2620	2790	3020
	(02)	150	175	220	230	250

The other facilities funded by Chemical Sciences are embedded in major laboratories and involve many interactions of scientists who are engaged to various degrees in other research projects also. This makes it exceedingly difficult and time-consuming to ascertain separate funding figures for the embedded facilities.

4. **For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Chemical Sciences funding going to DOE laboratories.**

Answer: The Chemical Sciences funds going to DOE Laboratories are:

FY 1981

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
Ames	943	1465	2388	171	0
ANL	5759	2270	8029	750	0
BETC	0	160	160	10	0
BNL	7228	2190	9418	904	0
INEL	0	100	100	5	0
LANL	85	630	715	55	0
LBL	3165	1240	4405	370	3000
LLNL	0	310	310	25	0
MOUND	0	950	950	65	0
NOTRE DAME	2232	0	2232	190	0
ORNL	1595	5415	7010	535	200
PETC	0	61	61	5	0
PNL	0	1235	1235	85	0
SNLA	145	100	245	10	0
SNLL	4000	150	4150	800	38
SERI	320	50	370	20	0

FY 1982

	(K$, Operating) Budget Category	(K$)			
	01	02	Total Op.	Equip.*	Const.*
Ames	1025	1640	2665	403	0
ANL	6755	2565	9320	880	0
BETC	0	153	153	0	0
BNL	10615	1780	12395	1303	300
INEL	0	120	120	15	0
LANL	95	775	870	60	0
LBL	3790	1625	5415	470	0
LLNL	0	240	240	15	0
MOUND	0	916	916	60	0
NOTRE DAME	2232	0	2325	290	25
ORNL	1644	5776	7420	510	0
PETC	0	95	95	5	0
PNL	0	1128	1128	75	0
SNLA	140	170	310	20	0
SNLL	4270	175	4445	975	0
SERI	430	100	530	35	0

FY 1983

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
Ames	930	1882	2812	335	0
ANL	7400	3213	10613	885	300
BETC	0	170	170	12	0
BNL	10785	1770	12555	1383	100
INEL	0	165	165	12	0
LANL	0	715	715	52	0
LBL	4296	1740	6036	918	0
LLNL	0	184	184	13	0
MOUND	0	978	978	71	0
NOTRE DAME	2663	0	2663	193	0
ORNL	1640	6085	7725	562	0
PETC	0	80	80	6	0
PNL	0	1300	1300	90	0
SNLA	150	260	410	29	0
SNLL	4790	20	5010	905	0
SERI	450	150	600	44	0

FY 1984

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
AMES	910	2036	2946	447	0
ANL	7834	3513	11347	1105	100
BETC	0	177	177	15	0
BNL	11973	1854	13767	1491	0
INEL	0	120	120	11	0
LANL	0	719	719	64	0
LBL	4411	1717	6128	1071	0
LLNL	30	0	30	3	0
MOUND	0	950	950	71	0
NOTRE DAME	2835	0	2835	252	0
ORNL	1658	6058	7716	691	250
PETC	0	93	93	7	0
PNL	0	1310	1310	116	0
SNLA	155	500	655	58	0
SNLL	5280	229	5509	800	100
SERI	575	156	731	65	0

FY 1985

	(K$, Operating) Budget Category			(K$)	
	01	02	Total Op.	Equip.*	Const.*
AMES	925	2205	3130	450	600
ANL	8235	3531	11766	3475	5200
BETC	0	186	186	22	0
BNL	13170	1819	14989	1303	100
INEL	0	126	126	15	0
LANL	0	504	504	60	0
LBL	4455	1670	6125	731	0
LLNL	45	0	45	0	0
MOUND	0	730	730	81	0
NOTRE DAME	3005	0	3005	359	50
ORNL	1725	6206	7931	846	0
PETC	0	87	87	10	0
PNL	0	1419	1419	169	0
SNLA	165	368	533	64	0
SNLL	5750	250	6000	700	0
SERI	675	164	839	100	0
SSRL	0	0	0	0	100

* Capital equipment and construction funds are not apportioned by category below the subprogram level.

5. **For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of Chemical Sciences funding going to universities.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
CHEMICAL SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0301 FUNDAMENTAL INTERACTIONS					
OPERATING EXPENSES					
ALABAMA A&M UNIV	$ 0	$ 0	$ 0	$ 100	$ 0
ALABAMA UNIV OF	53	58	63	67	71
ARIZONA UNIV OF	122	131	196	77	173
ARKANSAS UNIV OF	37	40	0	42	48
BOSTON UNIV	368	88	435	75	272
BRANDEIS UNIV	80	96	90	95	100
BROWN UNIV	64	112	125	147	156
CALIF UNIV OF BERKELEY	80	88	0	80	0
CALIF UNIV OF DAVIS	64	60	48	0	0
CALIF UNIV OF IRVINE	222	200	170	180	192
CALIF UNIV OF LOS ANGELES	77	150	92	100	105
CALIF UNIV OF SAN DIEGO	0	55	61	64	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
CALIF UNIV OF SANTA BARBARA	208	241	135	121	163
CALIFORNIA INST OF TECH	200	212	222	236	250
CARNEGIE MELLON UNIV	0	60	60	50	0
CHICAGO UNIV OF	215	215	229	217	222
CLARKSON COLLEGE OF TECH	0	60	68	155	0
CLEMSON UNIV	0	110	0	65	0
COLORADO UNIV OF	268	180	264	267	288
COLUMBIA UNIV	68	220	35	160	70
CONNECTICUT UNIV OF	3	0	0	0	0
CORNELL UNIV	154	50	242	179	190
DARTMOUTH COLLEGE	0	0	82	0	41
DREXEL UNIVERSITY	110	0	55	60	0
FLORIDA STATE UNIV	42	0	0	0	0
FLORIDA UNIV OF	56	60	65	71	75
GEORGIA INS OF TECHNOLOGY	54	55	60	66	70
GEORGIA UNIV OF	0	0	48	54	60
HARVARD UNIV	79	90	95	100	108
HEBREW UNIV	11	0	0	0	0
HOUSTON UNIV OF	0	160	0	90	95
HOWARD UNIV	47	47	50	55	56
ILLINOIS INST TECH	136	136	169	177	190
ILLINOIS UNIV OF	151	160	165	177	190
JACKSON STATE UNIV	0	0	50	55	60
JOHNS HOPKINS UNIV	192	0	65	68	72
KANSAS STATE UNIV	543	634	625	676	734
KANSAS UNIVERSITY OF	124	130	144	154	166
KENTUCKY UNIV OF	45	48	0	0	0
LOUISIANA STATE UNIV	132	25	70	117	123
MASSACHUSETTS INST TECH	300	313	351	382	404
MASSACHUSETTS UNIV OF	116	0	66	0	76
MINNESOTA UNIV OF	403	334	264	250	162
MISSOURI UNIV OF	62	68	65	72	78
MOREHOUSE COLLEGE	0	0	44	48	0
MOUNT HOLYOKE COLLEGE	56	114	0	65	0
NEBRASKA UNIV OF	188	140	215	220	230
NEW MEXICO UNIV OF	88	97	90	105	110
NEW ORLEANS UNIV OF	50	47	55	60	64
NEW YORK ST UNIV OF BROOKLYN	60	57	62	64	68
NEW YORK ST UNIV OF ST BROOKE	52	52	74	65	70
NEW YORK UNIV	80	0	80	90	90
NORTH CAROLINA UNIV OF	270	152	237	259	281
NORTHWESTERN UNIV	46	48	0	0	0
NOTRE DAME UNIV OF	2232	2450	2663	2835	3005
OHIO STATE UNIV	215	62	142	104	0
OKLAHOMA UNIV OF	100	86	86	0	0
OREGON GRADUATE CENTER	0	0	90	0	70
OREGON STATE UNIV	45	45	0	0	0
OREGON UNIV OF	45	7	29	0	0
PENNSYLVANIA STATE UNIV	88	91	127	104	110
PITTSBURGH UNIV OF	0	- 8	0	0	0
PRINCETON UNIV	208	78	282	309	335
PUERTO RICO UNIV OF	0	45	125	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
PURDUE UNIV	208	142	146	163	185
RENSSELAER POLYTECHNIC	0	0	80	85	85
RICE WILLIAM MARSH UNIV	279	298	356	458	275
ROCHESTER UNIVERSITY OF	109	116	125	330	149
SERI UNIVERSITY PGM	500	0	0	0	0
ST JOHN FISHER COLLEGE	0	109	0	60	0
STANFORD LELAND JR UNVR	260	277	98	422	151
TEMPLE UNIV	130	0	67	80	0
TENNESSEE UNIV OF	130	135	134	141	149
TEXAS A & M UNIV	160	118	65	70	75
TEXAS UNIV OF	125	130	68	144	80
TOLEDO UNIV OF	0	21	55	0	32
UTAH UNIV OF	148	153	214	186	85
VANDERBILT UNIV	59	72	78	82	88
WASHINGTON UNIV ST LOUIS	81	85	86	93	90
WAYNE STATE UNIV	149	142	76	77	0
WESTERN MICHIGAN UNIV	0	0	37	55	65
WILLIAM & MARY COLL OF	65	72	75	80	85
WISCONSIN UNIV OF	130	21	22	94	70
WORCESTER POLYTECH INST	78	0	43	0	0
WRIGHT STATE UNIV	135	138	55	59	65
YALE UNIV	63	63	63	68	75
KC0302 PROCESSES AND TECHNIQUES					
OPERATING EXPENSES					
AMHERST COLLEGE	41	47	47	49	50
ARIZONA UNIV OF	66	71	74	82	81
BRIGHAM YOUNG UNIV	212	194	251	213	228
BROWN UNIV	83	55	58	62	65
CALIF UNIV OF DAVIS	65	145	0	82	85
CALIF UNIV OF IRVINE	72	75	141	153	158
CALIF UNIV OF LOS ANGELES	189	183	195	200	205
CALIF UNIV OF SANTA BARBARA	108	118	130	136	142
CALIFORNIA INST OF TECH	71	188	46	159	168
CHICAGO UNIV OF	60	60	81	156	87
COLORADO STATE UNIV	112	52	125	138	145
COLORADO UNIV OF	27	235	0	135	134
COLUMBIA UNIV	66	138	147	250	164
CONNECTICUT UNIV OF	0	0	51	54	56
CORNELL UNIV	70	250	50	115	105
FLORIDA UNIV OF	0	0	4	0	0
GEORGE WASHINGTON UNIV	0	0	0	58	70
GEORGIA UNIV OF	139	168	77	155	148
HARVARD UNIV	47	0	0	0	0
HOUSTON UNIV OF	145	160	164	168	174
HOWARD UNIV	0	0	- 5	0	0
ILLINOIS INST TECH	54	0	- 3	0	0
ILLINOIS UNIV OF	0	0	0	124	0
INDIANA UNIV	230	44	262	54	209
JOHNS HOPKINS UNIV	40	56	81	75	80

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KENT STATE UNIV	54	60	57	66	0
KENTUCKY UNIV OF	140	0	70	0	0
LEHIGH UNIV	0	0	297	86	115
MARQUETTE UNIV	44	105	0	60	63
MARYLAND UNIV OF	95	108	107	0	0
MASSACHUSETTS INST TECH	0	93	373	53	205
MASSACHUSETTS UNIV OF	70	0	60	0	0
MINNESOTA UNIV OF	180	185	220	215	227
MISSOURI UNIV OF	7	0	64	65	71
NEBRASKA UNIV OF	60	90	- 16	63	0
NEW YORK CITY U - BROOKLYN	0	0	- 5	0	0
NEW YORK CITY U	0	0	80	80	60
NEW YORK ST UNIV OF ST BROOKE	412	260	322	146	260
NORTH CAROLINA STATE U	64	0	0	0	0
NORTH CAROLINA UNIV OF	65	60	68	70	74
NORTHWESTERN UNIV	234	270	155	338	347
OHIO STATE UNIV	63	72	- 2	0	0
OKLAHOMA UNIV OF	0	0	0	65	63
PENNSYLVANIA STATE UNIV	302	258	283	382	341
PENNSYLVANIA UNIV OF	0	0	84	169	179
PITTSBURGH UNIV OF	125	187	234	221	226
PURDUE UNIV	130	75	137	137	146
RENSSELAER POLYTECHNIC	0	83	185	0	100
ROCHESTER UNIVERSITY OF	0	0	60	66	73
RUTGERS UNIV	84	63	5	0	0
SAN DIEGO ST UNIV FDT	0	0	60	65	68
SOUTHERN CAL UNIV OF	60	60	0	0	0
STANFORD LELAND JR UNVR	323	193	304	166	292
SYRACUSE UNIV	164	164	241	324	328
TENNESSEE UNIV OF	0	0	107	109	107
TEXAS A & M UNIV	255	135	224	156	165
TEXAS SOUTHERN UNIV	46	27	0	0	0
TEXAS TECH UNIV	43	43	112	91	125
TEXAS UNIV OF	125	0	55	53	57
UTAH UNIV OF	142	312	165	337	281
VERMONT UNIV OF	46	0	0	0	0
VIRGINIA UNIV OF	59	63	73	64	67
WASHINGTON STATE UNIV	60	60	0	75	0
WASHINGTON UNIV OF	0	0	0	70	75
WAYNE STATE UNIV	0	65	84	83	88
WEBER STATE COLLEGE	55	45	0	0	0
WESLEYAN UNIV	115	0	- 45	0	0
WISCONSIN UNIV OF	0	170	0	97	101
WYOMING UNIV OF	63	67	77	77	81
YALE UNIV	296	211	185	310	333
35KC03 CHEMICAL SCIENCES					
CAPITAL EQUIPMENT					
NOTRE DAME UNIV OF	190	290	193	252	359

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
39KC00 CHEMICAL SCIENCES					
CONSTRUCTION					
KANSAS STATE UNIV	0	0	0	0	2000
NOTRE DAME UNIV OF	25	25	25	0	50

6. **For the period FY 1981 - FY 1985, please provide, by budget category and by company, the amount of Chemical Sciences funding going to industry.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
CHEMICAL SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC03 CHEMICAL SCIENCES					
KC0301 FUNDAMENTAL INTERACTIONS					
OPERATING EXPENSES					
AEROCHEM RSRCH LABS INC	$ 85	$ 85	$ 71	$ 0	$ 0
CALSPAN CORPORATION	60	0	0	0	0
DYNAMICS TECHNOLOGY INC	79	80	0	0	0
SURFACE ANALYTIC RESEARCH	0	63	62	0	0
TECHNASSOCIATES INC	- 19	0	0	0	0
KC0302 PROCESSES AND TECHNIQUES					
OPERATING EXPENSES					
BEND RESEARCH INC	70	74	91	90	93
CALSPAN CORPORATION	0	0	49	62	68
FORD MOTOR CO	38	0	0	0	0
OWENS ILLINOIS INC	170	0	81	85	90
ROCKWELL INTER. CORP.	160	155	158	0	0

7. **For the period FY 1981 - FY 1985, please provide, by budget category and by agency, the amount of Chemical Sciences funding going to other agencies.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
CHEMICAL SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0301 FUNDAMENTAL INTERACTIONS					
OPERATING EXPENSES					
NAT BUREAU OF STANDARDS	$ 382	$ 509	$ 620	$ 662	$ 500
U.S. DEPT OF COMMERCE	0	0	19	0	0
KC0302 PROCESSES AND TECHNIQUES					
NAT BUREAU OF STANDARDS	397	542	510	537	582
NAVAL RESEARCH LAB	65	69	0	0	0

8. **How much of the FY 1985 Chemical Sciences budget request is for support of programs formerly funded by the DOE Nuclear Program or by any other DOE program?**

Answer: None.

9. **What new initiatives and expansion of current activities were recommended by the recent National Academy of Sciences Workshop on the Future of Transplutonium Element Research?**

Answer: The Workshop recommended that the High Flux Isotope Reactor (HFIR) and the Transuranium Processing Plant (TRU) be continued in operation for at least several years and then reviewed again. The reasons given for continuation were that (1) there is broad interest in areas of scientific research which depend critically on transplutonium elements and isotopes uniquely produced by the HFIR/TRU and (2) the facilities are also important for training, for research on fuel processing, for neutron scattering and for medical and defense applications. No distinctly new intiative was recommended, but the report urged that "the highest priority in research with transplutonium materials should be given to the support of these experimental programs identified in the panel reports as particularly interesting, promising, and crucially dependent on products of the HFIR/ TRU." A specific recommendation by one of the panels was that there be a tenfold increase in production of einsteinium-254 for use in the research seeking the superheavy elements.

Also suggested is consideration of expanding the Calutron operation for production of some rare isotopes of americium, curium and californium for studies of their nuclear properties.

Extending condensed-matter spectroscopy to the heavier transplutonium elements was suggested. Solid state physics and chemistry of the fifteen actinide elements should be expanded, the report suggested.

Each of the above panel recommendations would require additional funding and as a result we are considering these recommendations in light of overall Department budget priorities.

10. What have been the major accomplishments of this subprogram over the past five years?

Answer: From the many scientific accomplishments achieved with support from Chemical Sciences, selections were made from those which appear to be the most significant. Time often alters such judgments as unexpected turns take place in science, technology, commerce and opinion. Those selected follow.

Water Photolysis Process Yielding Hydrogen and a Stable Oxygen Species

A photolytic process of probable interest for industrial application has been discovered, yielding gaseous hydrogen and trapping the active oxygen simultaneously produced, in a stable form. Photolytic reactions induced by sunlight in water normally yield atomic hydrogen and oxygen-containing species such as the hydroxyl radical. The hydrogen atoms produced combine to form gaseous molecular hydrogen, but if the oxygen-containing species is not readily removed from the system, or if it does not readily react to produce gaseous oxygen, the production of hydrogen will soon terminate. In water splitting as in many other chemical reactions, the inability to remove a product from a reacting system often results in the buildup of species that initiate undesirable reverse or side reactions in the system. What has been discovered is a reacting system that overcomes this difficulty -- i.e, the oxygen-containing species is not a problem but a desirable product -- and should permit the development of a continuous photolytic process yielding hydrogen and usefully combined oxygen.

(Lawrence Berkeley Laboratory)

Catalyst Regeneration for Coal Gasification

Research has provided new insight into the poisoning by sulfur of the metal catalysts used for the methanation step of coal gasification. With this new insight also has come the demonstration that poisoned catalysts can be regenerated far more completely than current practice achieves. This may significantly improve economics of these catalyst systems for coal processing by extending the useful life of the catalysts and increasing the plant operating factor.

The usual regeneration practice for removal of the chemisorbed sulfur has been to heat the catalyst in air in order to oxidize the sulfur to gaseous sulfur dioxide. Since the catalyst surface also becomes oxidized and catalytically inactivated, normal practice has been to follow up with a hydrogen treatment which removes the oxygen. With the air treatment, however, an undesired oxidation of the metal surface proceeds faster than the desired oxidation of sulfur, which results in "buried" sulfur under the newly formed layers of metal oxide. The competing oxidation rates can be manipulated to favor oxidation of sulfur over that of metal, by drastically lowering the oxygen concentration to 1-10 parts per million and by carefully controlling the temperature. The catalyst, regenerated in this way, regains nearly 100 per cent of its original activity. The concept may be applicable to catalytic systems which are poisoned by sulfur.

(University of Delaware)

Catalyst Using Synthesis Gas as a Reducing Agent

Molecular hydrogen is required in many chemical processes involving reactions carried out through catalysis. However, the production of large quantities of chemically pure hydrogen is energy-consuming and expensive. A homogeneous rhodium carbonyl catalyst system which allows direct utilization of synthesis gas (mixture of CO and H_2) as a reducing reagent in place of molecular hydrogen for a specific class of reactions has been discovered. Synthesis gas is the principal product of the gasification of coal or char; it is a mixture of carbon monoxide and hydrogen of widely varying composition depending on the conditions used. Current practice requires further processing and separations to obtain hydrogen for use as a reducing agent. The catalytic reduction discovered proceeds by consuming both the CO and H_2 in proportion to their initial concentrations, thus allowing for the direct utilization of any composition of synthesis gas. The catalytic reduction reactions found are applicable in a number of industrial processes including production of plastics and some of the manmade fibers.

(University of Texas)

Production of Highly Charged Ions for Fusion-Related Research

The study of highly charged ions -- atoms which have been stripped of most of their electrons -- is important to development of fusion energy because these ions may occur in fusion plasmas and dramatically reduce their energy. Until now obtaining such highly stripped ions for laboratory research on their properties was possible only in energy ranges far above those typical of fusion plasmas. A new method has been devised which overcomes this problem. It involves a beam of particles at millions of electron volts striking a gas target and stripping the gas molecules of most of their electrons. The resulting highly charged ions emerge from the target at relatively low energies, only a few tens of electron volts, an energy range heretofore not attainable for such highly charged ions. The ions are then accelerated to a few hundred electron volts for the fusion-related experiments. This technique is being adopted by several laboratories.

(Kansas State University)

Sulfur Dioxide and Nitrogen Oxides Effect on Atmospheric Levels of Carbon Monoxide

Recent measurements of the isotopic (oxygen-18/oxygen-16) ratio in atmospheric carbon monoxide (CO) indicates a relatively large increase of technologically produced CO during this past 8 years. This increase, from 1971 to 1979, is by an amount greater than that attributable to the largest sources of technological CO, the internal combustion engine (IC). Two possible explanations are: (1) a large increase from biomass burning which Produces CO difficult to distinguish from ICE carbon monoxide or (2) a decrease in the atmospheric concentration of hydroxyl free radicals (OH) which are the principal scavengers of CO from the atmosphere. The first explanation does not seem very likely since patterns of biomass combustion have not changed dramatically during the past 10 years. The second possibility is disturbing, particularly if the reduction of OH radicals in the atmosphere were caused by an increase in the pollutant trace-gas scavengers for OH, such as sulfur dioxide and the nitrogen oxides.

(Argonne National Laboratory)

Palladium from Nuclear Waste

A technology for recovery of stable palladium during the reprocessing of nuclear fuel elements has been devised. Its implementation could ease our current heavy dependence on Soviet and South African palladium for automobile exhaust cleanup catalysts, and possible future use as a coal conversion catalyst.

The crux of the process is a strongly radiation-resistant system which enables the processing of spent nuclear fuel after a minimum of cooling time. The object is to remove fission product ruthenium as soon as possible. This ruthenium has a relatively short half-life of about one year, decaying into 30-second rhodium which decays to stable palladium-106. The required radiation-resistant system involves a high temperature chemical partitioning between molten uranium and magnesium. In this system, the required initial separation of ruthenium from the also-present radioactive palladium, with a separation factor greater than ten thousand, has been demonstrated. The stable palladium-106 is ultimately recovered free of radioactivity.

The U.S. production of palladium has never exceeded 1,000 kg per year while the consumption has reached 46,000 kg/yr. It is estimated that an annual production of about 1,000 kg is possible from reactors now operating or under construction.

(Oak Ridge National Laboratory)

Energy Efficiency in Natural Systems Leads to New Thermodynamic Insight

Research on the mechanism of an important biochemical process has provided new thermodynamic insight into the possibility of attaining greater efficiency of energy utilization in complex chemical systems.

Living systems derive their energy supply from the conversion of ATP (adenosine triphosphate) to ADP (adenosine diphosphate). ADP is converted back to ATP during glycolysis, the process which converts sugars to oxidized chemicals via a multi-step (9 or more) reaction pathway. The concentrations of the intermediates in the glycolysis process are observed to oscillate, with frequencies on the order of 1 minute, with definite relationships among the different intermediates' concentrations and their frequencies.

A description of the thermodynamics of reactions in systems where intermediate species concentrations oscillate has been developed. It demonstrates that oscillations in the multi-step glycolysis sequence result in an increase of 10-15% in overall efficiency over that which would otherwise be observed. Essentially, this comes about because some of the energy which would be dissipated as heat is intercepted at peaks in the oscillations, and appears as useful chemical energy. Although developed to explain the biochemical phenomenon observed, the description has been recast to provide additional insight into the thermodynamics of a heat (Stirling) engine as an example of the generality of this concept.

(Stanford University)

Fluoroxysulfates: Powerful New Oxidants and Fluorinating Agents

A group of powerful oxidants and fluorinating agents which may prove to be uniquely useful synthetic and analytical tools for both inorganic and organic chemistry has been prepared, isolated and characterized. These are the first known ionic hypofluorites, or specifically, in this case, fluoroxysulfate (SO_4F^-) salts. The ionic character of these salts contributes to their relative stability. It is this stability and the ease of formation of these salts which make this new kind of reagent so potentially attractive. The fluoroxysulfate salt of rubidium or cesium separates out as a solid when fluorine gas is passed through a water solution of rubidium or cesium sulfate. Earlier, other chemists had noted that passing fluorine through aqueous sulfate solutions gave a powerful oxidant which decomposed in a few hours, but this observation had been largely ignored and even questioned before this recent work.

(Argonne National Laboratory)

New Analytical Techniques Using Fiber Optics Devised

A novel application for fiber optics may soon find many uses. A linear array has been assembled of 30 fibers (the number could be greater) with lengths varying from 1 to 59 meters, all leading into a single photomultiplier, a device which measures intensities of pulses of light. The 2 meter increment in length from one fiber to the next provides an incremental time delay of 10 nanoseconds (billionths of a second) between the pulses received by the photomultiplier from each fiber. A nanosecond pulse of light is spread by a diffraction grating into 30 different wavelength groups and each of these is focused on the receiving end of one of the 30 optical fibers. These all lead to the single photomultiplier, so that its output is a series of 30 electrical pulses, 10 nanoseconds apart, with intensity corresponding to the intensity of the light within the wavelength range of each fiber's placement.

The system can be tailor-made to monitor, as a function of time, the particular spectral range of interest in specific analytical applications. In practice it would compare a blank with a sample interposed between the light source and the diffraction grating, thus providing a fast, accurate analytical reading.

(Oak Ridge National Laboratory)

Laser Based Technique Permits Study of Critical Trace Species in Flames

Saturated absorption spectroscopy, a new laser-based technique is being used to study some of the less well understood aspects of combustion. A flame can be scanned to measure the location and concentration of highly dilute chemical species that are difficult, if not impossible, to detect by other means. This new technique holds promise for identifying and understanding the roles of dilute, but highly reactive species believed to be important in combustion. The technique uses crossed laser beams, to define a small volume element (essentially a point) within the flame. One beam is much more intense than the other. At a proper choice of wavelength the intense beam excites a large fraction of the species under study to an energy level

characteristic of that species. The second beam, of the same wavelength, is much lower in intensity. If one measures absorption of the second beam when the first beam is off and then on, one finds a decrease which is proportional to the number of molecules excited by the first laser beam. Since the number of molecules excited is, in turn, proportional to the total number present, their absolute concentration can be determined after the process has been suitably calibrated.

(Sandia National Laboratory)

Highly Specific Extractants Synthesized for Recovery and Purification of Valuable Metals

Research started in 1980 has led to the discovery of bifunctional extractants for recovery and purification of actinides from nitric acid and from other nuclear waste solutions. They also can be used for recovery of certain valuable fission products, e.g. palladium, from high level liquid waste. This new class of bifunctional extractants, i.e. extractants which have two potential donor groups in the same molecule, are called carbamoylmethylphosphine oxides (CMPO). The carbamoyl and phosphine groups are connected by a methyl (CH_2) group. The nitrogen of the carbamoyl group has two organic groups attached to it as does the phosphorus in the phosphine group. By proper choice of these two sets of organic groupings it is possible to synthesize a CMPO which extracts americium from nitric acid solutions with a distribution coefficient greater than 20, that is, over 95% extraction efficiency. Tetra- and hexa-valent actinides are extracted with even higher distribution coefficients. Selectivity of actinides from practically all fission products is achieved by "scrubbing" with nitric acid-oxalic acid.

(Argonne National Laboratory)

New Photochemical Reaction for Producing Hydrogen

Sunlight, striking a photoelectrochemical cell containing a tungsten disulfide semiconductor electrode in a concentrated solution of sulfuric acid, will convert sulfur dioxide to sulfuric acid with the simultaneous formation of hydrogen. This photochemical reaction, which takes place with sunlight as the only energy source, occurs with 5% efficiency in normal sunlight and without degradation of the materials involved. This reaction is particularly interesting because of a known thermal reaction that decomposes sulfuric acid into sulfur dioxide and oxygen. The coupling of these two reactions would conserve sulfur dioxide and sulfuric acid; the result would be a reaction system using heat and sunlight to decompose water to hydrogen and oxygen without undesirable waste products. So far the reaction has been studied only with expensive single-crystal tungsten disulfide. Less expensive polycrystalline materials seem possible. The reaction of SO_2 to produce H_2SO_4 is also of considerable interest in the fertilizer industry.

(Massachusetts Institute of Technology)

Dynamics of Molecular Ions Now Accessible Through Controlled Coulombic Fragmentation

A new technique now permits the experimental determination of the structure and binding forces in molecular ions. These ions are extremely reactive species that can have profound effects on chemical reactions. This great reactivity has made it impossible to determine the structural and binding characteristics of molecular ions except in a few rare situations. The ion studied is accelerated and passed through a thin crystal, which gently strips electrons from the ions. This leaves constituent atoms positively charged, so that electrostatic repulsion breaks the ion apart. As the constituent charged atoms separate, the time and place of detection of these fragments are determined and can be used to calculate a series of "snapshots" of the ion as it disintegrates. This information in turn reveals the forces binding the atoms together in the ion. Among processes that can benefit from this knowledge are the direct conversion process in MHD and studies of energy loss mechanisms in fusion plasmas.

(Argonne National Laboratory)

Change in Catalyst Substrate Dramatically Changes Fuel Product

Preliminary experimental results have dramatically shown that the specificity of the catalytic conversion of coal synthesis gas ($CO + H_2$) to methanol and methane is dependent on the type of silica substrate used to support the palladium metal catalyst. Palladium on Grade-57 silica gel was almost 100% selective in catalyzing the formation of methanol whereas palladium on Grade-01 gel had 100% selectivity to methane. Palladium on Cab-O-Sil was found to produce both fuels. The significance of this discovery is the knowledge that the ability of the palladium to catalyze the synthesis of methanol is not an inherent, general property of the metal alone. This is one of the most dramatic examples known of a substrate effect in heterogeneous catalysis. Research is in progress to explain this observation, which may strongly influence the use of synthesis gas from coal.

(Texas A&M)

Coal and Oil Shale Non-Destructively Analyzed for Organic Water

Valuable samples of coal solutions and oil shales were subjected to rapid nondestructive tests based on small angle scattering of neutrons. One objective was to learn if this technique could be used to physically characterize the samples prior to other necessary, but destructive tests. Very useful results were obtained: the concentration of coal in solution could be measured over a dynamic range of 10 and the size and shape distribution of pores in oil shale determined. Contrary to earlier assumptions, it was learned that the pores did not flatten with increasing lithostatic pressure (depth). Indeed, there does not seem to be a clear correlation between pore size and depth with means that specific site-depth testing is required before deciding how to extract oil from shale on a large scale basis. The neutron technique is extremely efficient requiring only a few hours for a full analysis and can cover a wide range of solution concentrations and pore configurations.

(Oak Ridge National Laboratory)

Coated Semiconductor Electrode Improves Possibility of Electrochemical Solar Cell

A new technique has been developed for electrodepositing a polymer film of polypyrrole on a polycrystalline n-type silicon semiconductor electrode. The treated electrode was used as the anode (positive electrode) in a cell containing a water solution of iron salts and an ordinary metal cathode (negative electrode). Upon illumination with visible light the iron was oxidized at the anode and reduced at the cathode, so that with no net change in the solution, electricity flowed in an external circuit. Untreated electrodes corrode sufficiently in a few seconds of operation to stop the flow of electricity. Initial tests of these coated electrodes were run for 120 hours with little change in their performance. Tests of power conversion indicated a 3% conversion efficiency, about one third that of a solid state device employing polycrystalline silicon. The important characteristics of this coating are its complete coverage of the electrode (providing the protection) and its high electrical conductivity (providing a path for the flow of electricity). Current research is exploring the properties of the polypyrrole film, its use to protect other semiconductor electrodes and its use in fuel-forming photoelectrochemical cells.

Two Discoveries Strengthen Scientific Basis for Catalyst Design

A better understanding of the detailed bonding interaction between the transition metals which are used as catalysts and substrates for synthesis gas ($CO + H_2$) conversions has resulted from two recent scientific discoveries. In the first, convincing evidence has been obtained favoring one of three proposed mechanisms for hydrocarbon chain growth in Fischer-Tropsch synthesis. The results clearly indicate that the chain growth occurs by insertion of CH_2 species into a metal alkyl bond. This insight is an important contribution to the design of catalysts of high specificity for conversion of synthesis gas into longer chain hydrocarbons. In the second, recent work has resulted in a kinetic method for obtaining values of metal-carbon bond strengths. These are very important in catalytic reactions involving the formation or isomerization of hydrocarbons. It has recently been shown that a kinetic method can be used to obtain values for chromium-carbon bond energies. Values for the energies of bonds between chromium and hydroxyalkyl groups have been obtained by measuring both forward and reverse rates of alpha-hydroxyalkyl metal-carbon bond reactions. These particular bond energies are especially important since hydroxyalkyls are believed to be intermediates in catalyzed $H_2 + CO$ reactions which lead to hydrocarbon and oxygenated hydrocarbon products (Fischer-Tropsch synthesis).

(University of Texas)

Improvement in Sulfur Isotope Ratio Measurements Significant for Identifying Acid Rain Sources

Coal is plentiful but coal combustion pollutes the atmosphere. Sulfur contaminants form sulfur oxides upon burning which contribute in part to "acid rain." Sulfur emissions contain varying sulfur-32/sulfur-34 isotope ratios depending upon the source. The ratios are different for sulfur derived from microbial activity, geologic emissions, or fossil fuel combustion. Thus, the isotope ratio gives an indication of the source of the

pollutant. It has been difficult, however, because of the excessively long measurement times required, to use sulfur isotope ratio determinations for source identification. In a basic research program in analytical chemistry at the Idaho National Engineering Laboratory, scientists have discovered a technique to make faster and far more precise sulfur isotope measurements. A thousand-fold improvement has been achieved in measuring the sulfur-32/sulfur-34 isotope ratio. Previous measurements had been made by positive ion mass spectrometry. In the new technique, sulfur oxides are caused to react with fluorine to form sulfur hexafluoride. Because this is a heavier compound which easily picks up electrons, it can be readily analyzed in a negative ion mass spectrometer. With the improved sensitivity, much shorter measurement times are required and thus determination of sulfur-32/sulfur-34 isotope ratios in air is feasible.

(Idaho National Engineering Laboratory)

Experimental Observation of "Hot Carriers" Could Lead to Doubling Efficiency of Photoelectrochemical Solar Devices

Photoelectrochemical systems convert solar energy to electrical or chemical energy. Scientists have developed a number of promising photoelectrochemical systems but they are far too costly for the amount of energy output. Research is being carried out at the Solar Energy Research Institute (SERI) to understand fundamental properties of photoelectrochemical systems.

A phenomenon known as "hot carrier effects" has been observed experimentally for the first time in photoelectrochemical systems. Hot carriers had been known in semiconductor solids but it was doubted that they could exist at a solid/liquid interface. Hot carriers are electrons in semiconductors which have been formed with more energy than necessary to excite the charge across the band gap. (The band gap is the difference between certain energy levels characteristic of each semiconductor.) Ordinarily, such electrons become "thermalized", that is lose energy and assume the temperature of their surroundings, before being ejected into solution. As "hot carriers" they retain some of the excess energy as they go into solution. Thus, the theoretical maximum efficiency for solar photoelectrochemical energy conversion using hot carriers is 66%, while the maximum efficiency with thermalized carriers is 31%. In addition, hot carriers can initiate chemical reactions that thermal electrons cannot.

The knowledge that hot carriers can exist at semiconductor/liquid interfaces will be useful to SERI and other scientists who are working in this area for designing more efficient photoelectrochemical systems.

(Solar Energy Research Institute)

New, Organometallic Chemistry May Help Coal Conversion and Industrial Chemicals

Chemical studies have led to (1) long sought-for activation of carbon-hydrogen bonds in saturated hydrocarbons, brought about by insertion of a transition metal atom between the carbon-hydrogen pair of atoms and (2) selective oxygen atom transfer to unsaturated hydrocarbons. The former may be important to activating organic groupings in coal for conversion while

the latter suggests more energy efficient processes for making important chemical intermediates.

One of the greatest challenges in homogeneous transition metal catalysis involving hydrocarbons has been the activation of carbon-hydrogen bonds in completely saturated hydrocarbons. Recently, the first stable transition metal complex capable of carrying out direct intermolecular insertion of a metal center into carbon-hydrogen bonds of completely saturated hydrocarbons was discovered. An organometallic iridium hydride complex was prepared upon irradiation with ultraviolet light underwent loss of molecular hydrogen to generate a highly reactive iridium center that inserted rapidly into the C-H bond of various hydrocarbons including saturated ones. The products have been characterized by spectroscopic techniques. Work is continuing on these reactions with attempts to develop catalytic processes for the conversion of hydrocarbons into other, more highly functionalized, organic molecules. This may be important to the activation of organic moieties in coal.

BES chemists have achieved an advance which could possibly lead to three-fold benefits in the chemical industry: large savings of energy and expense, much less wasteful use of petroleum for petrochemicals and the production of desirable chemicals which were previously difficult to obtain. These chemists have recently succeeded in preparing some palladium nitro complexes that are catalysts for the selective oxidation of various olefins to ketones or epoxides, which are important industrial chemical intermediates. The advantage of selective oxidation is that it overcomes inefficiencies in use of petroleum derived starting materials that stem from non-selective transfer of oxygen atoms from molecular oxygen to organic molecules in the catalytic cycle. A mechanism has been established for the ketone-producing catalytic cycle. It involves coordination of the olefin by palladium, transfer of an oxygen atom from the nitro complex to the olefin, separation of the product ketone and palladium nitrosyl complex and oxidation of the nitrosyl complex back to a nitro group by molecular oxygen.

(Lawrence Berkeley Laboratory and Brookhaven National Laboratory)

Experiments Impact Widely Held Theory by Showing Reaction of Oxygen Atoms With Unsaturated Hydrocarbons Does Not Involve Carbon-Carbon Bond Breakage

A turnabout has been forced on our understandings of an important aspect of combustion chemistry. Molecular beam experiments, supported by theoretical calculations, indicate that the reaction of oxygen atoms with unsaturated hydrocarbons leads preferentially to the formation of reactive species in which the oxygen atom has taken the place of another group in the molecule. Contrary to previous belief, carbon-carbon bond breaking does not occur.

Experimental investigation, under single collision conditions, of the reaction of unsaturated hydrocarbons and oxygen atom has indicated that the dominant reaction is the formation of a free radical in which oxygen atom substitutes for another group on a carbon atom in the hydrocarbon molecule. This is contrary to previously held opinions, based on cruder experiments, that the initial step in the reaction is the breaking of a carbon-carbon bond. This research was carried out with crossed molecular beams and experiments have been performed on a number of unsaturated hydrocarbons. Theoretical calculations done in the same laboratory on the ethylene-oxygen

atom reaction completely support the new experimental conclusions. These new results alter our ideas concerning the mechanism of hydrocarbon oxidation with important implications for modeling hydrocarbon combustion. The research was performed by Y. T. Lee, a recent Lawrence Award winner and his collaborators.

(Lawrence Berkeley Laboratory)

Molecular Clusters Generated Having Hundreds to Thousands of Molecules Bearing a Single Unit of Electric Charge

Nuclear fusion has the theoretical potential to create large amounts energy with small amounts of raw material. The science, however, is still in its early stages of development, and although much progress is being made along promising routes, it is still worthwhile to explore other avenues. In a basic research program on mass spectrometry at the Brookhaven National Laboratory, a possible new approach to fusion has been conceived. The project is jointly funded by the Division of Chemical Sciences and the Division of Advanced Energy Projects.

Very large clusters of hydrogen molecules have been generated, each of which contains hundreds of thousands of molecules and one unit of electrical charge. These cluster ions are a new type of chemical species. Produced in a specially built mass spectrometer, they survive as long as they are not allowed to collide with other molecules. Because the clusters contain electrical charge, it should be possible to accelerate them in a properly designed ion accelerator. They can then be made to collide with solid targets or perhaps other cluster ions. This might lead to the creation of microplasmas at extremely high temperatures and thus to conditions needed for nuclear fusion.

(Brookhaven National Laboratory)

Major Advance in Atomic Physics Permits Spectroscopic Study of X-rays Produced at Instant of Collision of an Ion and an Atom

A major advance in atomic physics has opened up an entirely new area of study: quasimolecular x-ray spectroscopy. Highly energetic atomic ions are first slowed, then collided with target atoms. At the moment of collision, x-rays are produced that can be associated with neither projectile nor target species but with a short-lived "molecule" of the two. Spectroscopy of these will add to our understanding of processes important in fusion.

A BNL physicist reports that the study of low energy multiply charged ions using the accel/decel technique has opened up an entire new field of spectroscopy of quasimolecular x-rays in collision physics. Chlorine ions, each stripped of sixteen of its seventeen electrons and having an energy of 300 keV/amu, were directed into a gas target where collisions produced x-rays that were not identifiable as belonging to either one of the atoms participating in the collision. Instead, the x-rays emitted were identified with a quasimolecule that is formed and exists only for the period of the collision.

Previously, chlorine ions containing only one electron were produced at 4.5 MeV/amu, an energy so large that the x-rays emitted during collisions were greatly and asymmetrically broadened toward higher energy. This distortion obscured the process involving the transfer of electrons from one collision partner to the other. The x-ray structure observed at the higher energy made it impossible to assign a specific energy value to each of the x-rays produced and to detect the predicted oscillatory dependence of x-ray spectra on the impact parameter.

The new development permits a clear energy assignment to be made and allows for the oscillatory behavior to be documented. The better resolved spectra are necessary to understand the physics that takes place during the 10^{-18} sec collision which is 100 to 1000 faster than the transition lifetimes of x-rays emitted by the individual atom.

This development occurred as part of a research effort supported by Chemical Sciences in response to the needs of magnetic fusion energy technology where the physics associated with low energy highly charged ions are not well understood. The accel/decel proof-of-principle was demonstrated earlier by Jim Bayfield at the University of Pittsburgh, then under contract with the Division of Chemical Sciences. As far as is known, the BNL accelerator is the only unit in the world that can conduct this type of experiment. The only other possible competition may come from two laboratories in Germany (GSI and Heidelberg) but it is expected that they will require 3 to 4 years of development before they can obtain similar results. One of these laboratories, the one at Heidelberg, supported members of their staff to collaborate in the BNL experiments.

(Brookhaven National Laboratory)

Selective Catalytic Conversion of Metanol To Ethanol Discovered

A new catalyst system has been discovered for conversion of methanol to ethanol. The system has several practical advantages over existing methods. Starting with methanol produced from coal, dry ethanol, which has higher fuel value per unit volume than methanol, is produced. The catalyst is based on iron pentacarbonyl in the presence of a tertiary amine. The principal co-product formed is carbon dioxide, rather than water as in existing methods which use a cobalt/carbonyl catalyst. Eliminating water is particularly beneficial because it can save the costly drying step.

In addition to not producing water, the iron system catalyzed reaction only requires half as much expensive hydrogen as in the cobalt/carbonyl catalyzed system. The selectivity of the iron/amine catalyst is virtually 100% for converting methanol to ethanol. There are no higher alcohols, alkyl acetates or acetals formed, in contrast to the cobalt systems, and this simplifies product purification considerably.

A mechanism for the iron/amine catalyzed reaction has been established through detailed chemical and kinetic studies. This understanding has led to development of a mixed catalyst, $Mn_2Co_{10}Fe(Co)_5$/amine, which has both activity and selectivity superior to either metal carbonyl alone.

(Argonne National Laboratory)

New Thin Film Photoelectrode Uses Visible Light to Generate Electricity or Split Water

One micron films of intrinsic (updoped) amorphous hydrogenated silicon deposited on stainless steel have been investigated as photocathodes in photoelectrochemical cells. The hydrogenated silicon was synthesized at RCA and its behavior characterized at MIT. The photoelectrodes are rugged, efficient and inexpensive.

The efficiency of the photocathode for converting visible light to electricity is in the 1-2% range, which is only about one-third less than efficiencies attained using expensive single crystal electrodes under the same conditions. Even more promising is the observation that this type of electrode produced a photovoltage more than 50% greater than that produced using a single crystal electrode. The efficiency for generating hydrogen by photoassisted electrolysis of water is equal to that obtained with the best single crystal electrodes.

Many advances reported in photoelectrochemical energy conversion in the past two years have been obtained with use of ultraviolet light, a less intense part of the solar spectrum at the earth's surface. This set of advances, in contrast, used the much more abundant visible part of sunlight. Research continues to increase further both our scientific understanding of these phenomena and the efficiencies of functioning of the new type of electrodes.

(Massachusetts Institute of Technology)

Soot Formation at Elevated Pressures Studied Using Laser Probe

Using advanced laser diagnostic techniques, considerable advances are being made in understanding the complex phenomena involved in the behavior of flames. The formation of soot, the familiar particulate matter resulting from incomplete combustion, is not only a serious source of reduced efficiency during combustion, but a potential environmental hazard as well.

Although there have been extensive studies of soot formation in combustion systems, most investigations have been carried out at normal or atmospheric pressure, despite the fact that, in practice, soot formation is most often a problem in systems that operate at high pressure. Applying advanced laser techniques, direct evidence has been obtained that soot formation increases at high pressures, not because the particles become larger, but because there are more of them.

While flames at elevated pressure are similar to those at normal atmospheric pressure, they become more compact as pressure increases. It was found that, with increasing compactness of the flame under pressure, the number of soot particles formed increases considerably. The experimental evidence comes from the much greater reduction in intensity -- by a factor of about 400 -- of a laser beam as it passes through a soot laden flame at two and one-half atmospheres of pressure compared to a soot laden flame at normal atmospheric pressure. Particle size very much affects the scattering of the laser light, and the ability to distinguish between either larger particles or more particles being responsible for the reduced beam intensity is dependent on sophisticated scattering measurements and their interpretation.

This study is typical of those now permitted by the advanced techniques for combustion research available at the Combustion Research Facility and has produced some important insight into the fundamental mechanisms responsible for the increase in soot production with pressure. Results such as these will ultimately provide the understanding necessary to control soot production in practical combustion devices operating at elevated pressure.

(Sandia National Laboratories-Livermore, and Stanford University)

Highly Accurate Method for Isotope Ratio Measurements Devised Using Selective Ionization

A new, highly-selective method for measuring isotope ratios has been developed. The method, termed resonance ionization mass spectrometry (RIMS), is uniquely suited to the measurement of isotope ratios in situations where interferences from other elements are present. These interferences arise in mass spectrometry because ions are separated and detected according to mass. The problem of different atoms with the same mass occurs in both the lanthanide rare earths (.e.g., cerium, used in color TV tubes, and neodymium) and actinide elements (e.g., uranium and plutonium). Resonance ionization is very selective, producing ions of only one element at a time, thus removing interferences without resorting to chemical separations or artificial measurement conditions, which seriously impair precision.

Research thus far has focused on the system cerium:neodymium:samarium (Ce:Nd:Sm) because Nd is an important element in nuclear reactor fuel burnup analysis. Interferences from Ce (mass 142) and Sm (masses 144, 148 and 150) must be eliminated in order to arrive at an accurate isotopic analysis of Nd.

A high-powered nitrogen laser and a dye laser are used to produce light pulses of the proper wavelength to ionize Nd selectively in the presence of Sm and Ce. The ions thus formed are mass analyzed in a mass spectrometer. By switching the spectrometer back and forth between two masses, an isotopic ratio can be measured. The results obtained for isotopic ratios of Nd and Sm can be compared to the results from ordinary mass spectrometry taken under the same conditions. Errors of several hundred percent have been reduced to 1-2% with the new measurements!

(Oak Ridge National Laboratory)

Shear Added as a Variable to Equation of State for Fluids at Very High Flow

It has been found by techniques of molecular dynamics that in fluids, under conditions of very high flow, the equation of state includes a term involving shear as a parameter along with the usual variables of temperature, pressure and volume, necessary to define the intrinsic properties of a fluid.

Equations of state are used to predict the properties of fluids, including thermodynamic properties which are, in turn, used in the prediction of fluid behavior and the design of chemical processes. The discovery of the shear effect offers an explanation of previously unaccounted for observations of phase changes occurring under conditions of high shear. This discovery is

expected to make it possible to predict thermophysical properties of complex fluids under conditions of unusual shear. Heretofore, there has been no awareness of the "shear" term because it makes essentially no contribution in the equation of state under normal conditions. Under conditions of very high flow or extreme mixing of a fluid, shear is high enough to have an effect.

The consequence of the shear effect is illustrated by the nitrogen-ethane system in which a region of non-miscibility, or a miscibility gap, is predicted by "normal" theory at given conditions of temperature and pressure, but disappears entirely when shear is taken into account. The nonexistence of a miscibility gap has significant practical consequences.

(National Bureau of Standards)

Scientific Method Established for Assessing Hydrogen Donor Capacity of Solvents for Coal Liquefaction

A new procedure has been developed to assess how effective various solvents might be as sources of hydrogen in coal liquefaction. Liquefaction of coal involves breaking chemical bonds between carbon atoms and increasing the hydrogen content to establish more liquid-like properties in the system. Since well established chemical principles involving bond dissociation energies form the basis of the new procedure, it can be used reliably to guide the production of better hydrogen donor solvents.

In this new procedure, a reactive chemical fragment, the orthoallylbenzyl radical, is generated by thermally decomposing the chemical substance orthoallylazotoluene. In the presence of a hydrogen donor or coal liquefaction solvent, this radical can either abstract hydrogen from the donor solvent or undergo an intramolecular rearrangement reaction. The two processes form two very different hydrocarbon products. Measurement of the yield or concentration ratio of these two products allows direct comparisons to be made of the hydrogen donor capacity of potential coal liquefaction solvents: the greater the yield of the chemical resulting from hydrogen abstraction, the better the donor capacity of the solvent.

The hydrogen donors studied thus far show expected trends of greatly increased rates of abstraction as the bond dissociation energy of the donor compound drops. The method is currently being applied to a wide variety of donor molecules and is ideal for the characterization of hydrogen donor solvent quality.

(Pacific Northwest Laboratory)

Unexpectedly Fast Electron Transfer Across Large Molecules Discovered

A novel set of experiments has demonstrated that electrons move surprisingly fast across large molecules. The molecules were designed with a rigid bridge separating parts of the molecule that can accept electrons at fixed, known distances. In the experiment electrons generated in a linear accelerator attach themselves at one end of each molecule and the rate at which they move to the other end is measured. Because the measured rates are extremely fast, and the spacer region is an electron insulator, it was

determined electron transfer was accomplished by a "tunneling" or jumping mechanism. These results are of particular importance in the solar photochemistry research area where initial charge separation following absorption of light energy may be accomplished following such a jump.

(Argonne National Laboratory)

Elusive Energy Loss Process Affecting Fusion Verified

Measurements of dielectronic recombination, a process that has eluded experimenters for years, have finally been made. The dielectronic recombination cross sections for the doubly charged ion of boron were measured; that is the first time such measurements have been made for an ion with multiple charges.

Dielectronic recombination involves the loss of energy in a plasma and occurs when energy is absorbed by an ion when it captures an electron in the plasma. At the instant of capture, the positive charge on the ion is reduced by one unit and the resulting ion is left with excess energy. The ion next rids itself of the extra energy by the release of a photon most likely in the form of an x-ray. The net effect of all this is that the energy initially provided to effect a collision between two atoms and cause fusion of the two nuclei is instead lost through radiation. The process is important to the understanding of the behavior of plasmas and its measurement helps provide a more accurate account of the energy balance in a fusion plasma. This account in turn will permit the improved design of efficient fusion power plants.

The existence of the process was first suggested in the 1940's to account for observations made by astrophysicists to explain energy balance in stars. They could only observe the sum of several simultaneous processes, of which dielectronic recombination was one. Experimental study of the single isolated process was not possible. Now the process has been demonstrated by directing a beam of ions from an accelerator into a specially designed chamber filled with electrons. Close inspection of the interaction taking place in the chamber between the ions and electrons showed the effect sought.

While the first results are in some disagreement with theory, the fact that the process can now be studied experimentally is clearly a breakthrough in the field of high energy atomic physics and a significant contribution to our improved understanding of fusion plasma interactions.

(Oak Ridge National Laboratory)

Unexpected Photochemical Mechanism Discovered in Enzyme Process for Biomass Hydrogen Production

A new photochemical route to the utilization of photons for enzymatic dissociation of water to produce hydrogen from biomass has been discovered. Experimental measurements of the simultaneous generation of hydrogen and oxygen by a laser light saturation technique have established the unexpected insight that not all photodissociation of water occurs by the same photochemical mechanism. By examining the hydrogen to oxygen ratio, it was

apparent that the rate of hydrogen and oxygen generation was inconsistent with the time-accepted Z-scheme mechanism of photosynthesis. The hydrogen to oxygen ratio was found to be significantly below the 2:1 ratio of the water's composition, which suggested the existence of a chemical step that encumbers the release of hydrogen. The fact that a previously unexpected mechanism exists for the enzymatic dissociation of water in biomass systems has broad implications for future developments in solar photochemistry as well as in the case of biomass photolysis.

(Oak Ridge National Laboratory)

11. **For the period FY 1981 - FY 1985, how much funding has this subprogram provided and is estimated to provide for the R&D of experimental devices/apparatus?**

Answer: The advancing of scientific capabilities by R&D on experimental devices and apparatus is an integral part of most of the research efforts supported by Chemical Sciences. In most cases such R&D is intertwined with the scientific use of the apparatus, each feeding the other. It is therefore usually impossible to delineate funding for the R&D on devices/apparatus.

At the Combustion Research Facility, however, such a budgeting distinction has been made. The focus at CRF has been on lasers. New regions of laser power have been entered and new laser-based techniques have been devised. The funding of the R&D efforts at CRF for devices and apparatus follows this pattern:

(Budget Authority In Thousands)

FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
1,000	1,000	1,210	1,320	1,435

12. **How does the research funded by the Chemical Sciences subprogram differ, complement, supplement, or overlap chemistry research funded by other parts of DOE, as well as by other agencies such as the National Science Foundation and or the Office of Naval Research?.**

Answer: Research funded by Chemical Sciences seeks basic understanding which will serve as the knowledge pool in energy-related chemistry and atomic physics for present and future use. The chemical and atomic physical research programmed by Fossil Energy, Conservation and Renewable Energy, Nuclear Energy, Defense Programs and Fusion Energy is nearly all shorter term solving of problems for those technologies. For example, in a typical Chemical Sciences project related to fossil energy, researchers devise chemical routes to the synthesis of organometallic compounds of types which have been theoretically suggested as stages in the catalytic conversion of carbon monoxide to hydrocarbons. Fundamentally, this project tests catalytic theory by observing the organometallics' behavior. Better theory and other basic knowledge will lead to better coal conversion to liquid fuels.

A typical Fossil Energy project, on the other hand, works with a known catalyst to optimize its behavior in coal conversion by varying temperatures, pressures, catalyst makeup proportions, etc. Similarly, a Chemical Sciences project related to fuel conservation uses advanced laser techniques to get at the identity and rates of formation of fleeting but key molecular fragments in complex combustion sequences. A typical project supported under Conservation, on the other hand, would test the effects of catalysts on flame temperatures and composition of combustion product gases. Both Chemical Sciences' and the technological programs' projects hope to produce advances in energy technology: Chemical Sciences by new basic understanding and the technological programs by more immediate fixes.

Recently some of the Fossil Energy programs have moved in the direction of more basic research, which is to be encouraged because of the existing gaps between basic science and technological development. Often the scientists involved in Chemical Sciences research are associated with those involved in the technology programs, which stimulates and informs people in both types of effort. Other means similarly promote complementarity, including conferences of Chemical Sciences researchers in specific subjects to which are invited representatives of the DOE technology programs and others from pertinent industries. Exchange of program summaries and informal contacts also serve to foster complementarity and avoid duplication.

Other agencies such as the National Science Foundation and the Defense basic research agencies also support long range basic research. Here the differences are in overall program makeup: DOE's Chemical Sciences has its emphasis in energy-related areas, DOD's programs broadly serve defense areas of knowledge and the NSF seeks to maintain a balance of national scientific progress and capabilities. Information is exchanged by Chemical Sciences with those agencies in periodic meetings, by frequent telephone contacts and by listings of projects supported and proposed. Overlap is avoided except where needed to clarify contradictory interpretations.

13. What types of formal and informal advisory groups does the Division of Chemical Sciences employ to assure that the subprogram is of high quality and coordinated with the research carried out at other agencies? If any formal advisory groups exist, please define the role of each, and provide a listing of the current membership.

Answer: Formal advisory groups are not employed by the Division of Chemical Sciences. The Office of Basic Energy Sciences is exploring how best to obtain formal advice including that on the chemical sciences.

14. What is the current rate of Ph.D. production in the chemical sciences?

Answer: The National Academy of Sciences informs us as follows: the number of Ph.D.'s awarded in chemistry was 1,538 in 1980, 1,611 in 1981, and 1,678 in 1982. Doctorates awarded in chemical engineering numbered 285 in 1980, 296 in 1981 and 306 in 1982. We do not have readily available, comparable data for the flow of new doctorates arising from Chemical Sciences support.

15. What is the average cost to produce a Ph.D. in this field?

Answer: The only cost figure directly attributable to producing Ph.D.'s in the chemical sciences is salary or stipend paid to doctoral students. These fall in the $8,000-12,000 range, currently averaging about $10,000. Other costs are difficult to estimate in general, because of wide variations in professors' time absorbed, type and age of equipment used, supplies consumed, laboratory overheads, etc.

16. Has the number of chemical sciences researchers supported by this subprogram been increasing, stable, or decreasing over the past five years? What change will occur given the FY 1985 budget request?

Answer: The number of researchers supported by the Chemical Sciences subprogram has varied in the past five years, but not dramatically. Research projects supported numbered 344 in FY 1978, rose to 430 in FY 1980 and then declined to 389 in FY 1983. Among these, projects at DOE laboratories held in the 180's from 1978 to 1981 but dropped to 162 in 1983, mainly due to the funding impact of operating the National Synchrotron Light Source. Projects at other than DOE laboratories, predominantly at universities, have increased from 157 in FY 1978 to 230 in FY 1983. These trends will continue, given the FY 1985 budget request.

17. What is the average annual cost per year to this subprogram to support a chemical sciences researcher?

Answer: The average cost per year to this subprogram to support a chemical sciences researcher is $250,000.

18. Please provide a copy of the latest Chemical Sciences research summaries.

Answer: See attached.

Summaries of FY 1983 Research in the Chemical Sciences

September 1983

U.S. Department of Energy
Office of Energy Research
Division of Chemical Sciences
Washington, D.C. 20545

PREFACE

The purpose of this booklet is to inform those interested in research supported by the Department of Energy's Division of Chemical Sciences, which is one of six Divisions of the Office of Basic Energy Sciences in the Office of Energy Research.

These summaries provide to members of the scientific and technical public and interested persons in the Legislative and Executive Branches of the Government a means for becoming acquainted, either generally or in some depth, with the Chemical Sciences program. Areas of research supported by the Division are to be seen in the section headings, the index and the summaries themselves. Energy technologies which may be advanced by use of the basic knowledge generated in this program can be seen in the index and again (by reference) in the summaries.

Chemists, physicists, chemical engineers and others who are considering the possibility of proposing research for support by this Division will find the booklet useful for gauging the scope of the present program in basic research, and the relationship of their interests to the overall program. Proposals that expand this scope will also be considered or directed to more appropriate offices. The research program summarized here is intended to add significantly to the knowledge base on which successful energy technologies can grow. For this purpose, scientific excellence is a major criterion applied in the selection of research supported by Chemical Sciences. Another important consideration is the emphasizing of chemical, physical and chemical engineering subdisciplines which are advancing in ways which produce new information related to energy, needed energy data, or new ideas.

The program is distributed among several different kinds of performing organizations. About 50% of the projects take place at DOE laboratories, and half take place at universities and industrial laboratories. In DOE laboratories, most of the researchers are fully engaged in this work, while most university and industrial researchers necessarily divide their time among duties involving this research, other research, teaching responsibilities, etc. Thus, about 70% of the funding goes to Federal laboratories, 25% goes to the academic sector, and the remainder is at industrial and not-for-profit laboratories.

Questions about the details of the individual project may be directed to the investigators involved or the persons in charge at DOE Laboratories (who are identified at appropriate places in this booklet). Other questions about the program may be directed to the undersigned.

Elliot S. Pierce, Director
Division of Chemical Sciences
Office of Basic Energy Sciences

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*on leave from Lehigh University
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iii

Each Branch of the Division of Chemical Sciences is divided into programs which cover various disciplines. The following is a description of each of those programs. The staff members responsible for each program are indicated on page ii.

FUNDAMENTAL INTERACTIONS BRANCH (01-)

Photochemical and Radiation Sciences (01-01)

This program consists of research into the interactions of radiation with matter in all forms, but particularly with gases and liquids. A large part deals with the effects of ionizing radiation and fast electrons. The photochemical research is largely devoted to studies with visible radiation aimed at the capture and conversion of solar energy. This encompasses such fields as artificial photosynthesis, photoinduced electron transfer reactions in homo- and heterogeneous media, photoelectrochemistry, photocatalysi[, and the molecular storage of energy. A small part of the program is devoted to research in hot atom chemistry, i.e., the study of the effects of nuclear decay and the consequent release of energy on chemical reactions. A new and growing program of photochemistry, spectroscopy and related studies will be centered at the National Synchrotron Light Source at Brookhaven National Laboratory.

Chemical Physics (01-02)

Disciplines covered by this program include chemical dynamics, energy transfer, molecular structure and spectroscopy, theoretical quantum chemistry, and statistical mechanics.

Special emphasis is placed on basic research related to combustion; advanced diagnostic methods, spectroscopy, theory and the kinetics of elementary combustion reactions are of special interest. A major user-oriented facility, the Combustion Research Facility (CRF) at Sandia Laboratories/Livermore is supported by this program. This laboratory offers use of advanced instrumentation to interested combustion scientists from universities, industry and national laboratories.

Atomic Physics (01-03)

The Atomic Physics Program supports experimental and theoretical efforts associated with the study of atom and ion structures, energy levels and lifetimes of quantum states, and of transport and exchange processes characterizing transfer of energy, momentum and matter. These studies strive to attain the best and most complete basic knowledge of the properties and interactions of photons, electrons, atoms, ions and simple molecules. Continued emphasis of this research has been on the understanding of relatively high energy atomic physics that involves atoms stripped of all or most all electrons and of atoms and ions in which electrons are located at upper energy levels. Recent emphasis has been on the study of processes that lead to the production of coherent radiation and on the statistical properties of this radiation as they modify elementary atomic physics processes.

PROCESSES AND TECHNIQUES BRANCH (02-)

Chemical Energy (02-01)

This program includes basic chemistry research related to chemical transformations or conversions which are fundamental to new or existing concepts of energy production and storage. Of particular interest are those research activities with the objectives of understanding the chemical aspects of (1) catalysis, both heterogeneous and homogeneous, (2) the chemistry of fossil resources - particularly coal, including characterization and transformation, and (3) the conversion of biomass and related cellulosic wastes. The disciplines of organic, bio-, inorganic, physical, thermo- and electrochemistry including the more chemically oriented chemical engineering, are central to this program. The emphasis is on understanding the chemical principles underlying the new and developing technologies and on innovative chemical research with potential for new energy concepts.

Separations and Analysis (02-02)

The separations part of the program is directed at improving our basic understanding of methods for separating mixtures of gases, liquids, solids and their component molecules, cations, anions, and isotopes. The program covers a broad spectrum of separations concepts, including membrane processes, extraction at both standard and supercritical conditions, adsorption, chromatography, photodissociation, complexation, etc. The program is technique-oriented rather than species-oriented: i.e., the research involves elucidation of fundamental chemical phenomena for improved separations rather than developing specific processes for the separation of a particular species from particular matrices. The isotope separation program emphasizes isotopic properties and isotope effects and is very basic in nature.

The analysis part of the program is aimed at supporting research on analytical techniques where a better understanding of basic chemical phenomena may facilitate improvements in sensitivity, reliability, ease of operation and/or lower the costs of analytical determinations. Entirely new analytical techniques are also investigated, although this program does not support instrument development. New techniques are quickly reported in the literature so that those interested in instrument development can build on work supported herein. The program is not geared to using existing techniques to unravel the composition of samples nor to develop techniques to analyze particular chemical species or sample types. Rather it is aimed at obtaining a thorough understanding of the basic chemistry of an analytical technique so that others may use this understanding to improve its utility.

Chemical Engineering Sciences (02-04)

This program addresses the more scientific and energy-related aspects of chemically related engineering topics, including momentum and transport phenomena, thermodynamics and physical and chemical rate processes. Particular attention is given to turbulence research related to combustion; experimental and theoretical thermochemical and thermophysical properties, especially of mixtures, and phase equilibria, including supercritical extraction phenomena. Emphasis is given to improving and/or developing the scientific base for engineering generalizations and their unifying theories.

The following is a list of "persons in charge" of Chemical Science projects at DOE laboratories. These individuals are department/division, or laboratory administrators who can provide information about specific programs or refer inquiries to appropriate individuals.

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Chemical Sciences - Fundamental Interactions
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T Division
G. I. Bell - Phone: (FTS) 843-4401 or (505) 667-4401

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Table of Contents

DOE Laboratories

Photochemical and Radiation Sciences
- Ames Laboratory..... 1
- Argonne National Laboratory
  - Chemistry Division..... 2
- Brookhaven National Laboratory
  - Chemistry Department..... 5
  - Department of Applied Sciences..... 7
  - National Synchrotron Light Source..... 8
- Lawrence Berkeley Laboratory
  - Chemical Biodynamics Division..... 9
  - Materials and Molecular Research Division.....10
- Notre Dame Radiation Laboratory.....11
- Solar Energy Research Institute.....15

Chemical Physics
- Ames Laboratory.....16
- Argonne National Laboratory
  - Chemistry Division.....18
- Brookhaven National Laboratory
  - Chemistry Department.....19
  - Department of Applied Sciences.....21
- Lawrence Berkeley Laboratory
  - Applied Sciences Division.....21
  - Materials and Molecular Research Division.....22
- Oak Ridge National Laboratory
  - Chemistry Division.....25
- Sandia National Laboratories/Livermore.....26

Atomic Physics
- Argonne National Laboratory
  - Physics Division.....29
- Brookhaven National Laboratory
  - Physics Department.....31
- Lawrence Berkeley Laboratory
  - Materials and Molecular Research Division.....31
- Oak Ridge National Laboratory
  - Physics Division.....32
- Sandia National Laboratories/Albuquerque.....33

Chemical Energy
- Ames Laboratory.....34
- Argonne National Laboratory
  - Chemical Technology Division.....36
  - Chemistry Division.....36
- Bartlesville Energy Technology Center.....37

Brookhaven National Laboratory
Chemistry Department....38
Department of Applied Sciences....39
Lawrence Berkeley Laboratory
Applied Sciences Division....39
Materials and Molecular Research Division....40
Lawrence Livermore National Laboratory
Chemical Engineering Division....43
Los Alamos National Laboratory
CHM Division....43
INC Division....44
Mound Facility....44
Oak Ridge National Laboratory
Chemical Technology Division....45
Chemical Division....45
Pacific Northwest Laboratory
Chemical Technology Department....47
Pittsburgh Energy Technology Center....48
Sandia National Laboratories/Albuquerque....48
Solar Energy Research Institute....48

Separations and Analysis
Ames Laboratory....49
Argonne National Laboratory
Chemistry Division....51
Brookhaven National Laboratory
Chemistry Department....52
Department of Applied Sciences....52
Physics Department....53
Idaho National Engineering Laboratory....53,54
Los Alamos National Laboratory
P Division....54
Mound Facility....55
Oak Ridge National Laboratory
Analytical Chemistry Division....56
Chemical Technology Division....58
Chemistry Division....60
Pacific Northwest Laboratory
Biology and Chemistry Department....61
Chemical Technology Department....61
Radiological Sciences Department....62
Sandia National Laboratories/Albuquerque....63

Chemical Engineering Sciences
Lawrence Berkeley Laboratory
Applied Sciences Division....64
Materials and Molecular Research Division....64
Los Alamos National Laboratory
T Division....64
Oak Ridge National Laboratory
Chemical Technology Division....65
Sandia National Laboratories/Livermore....65

Offsite Contracts

Photochemical and Radiation Sciences....66
Chemical Physics....84
Atomic Physics....99
Chemical Energy....111
Separations and Analysis....129
Chemical Engineering Sciences....141

Equipment Funds....146

Special Facilities....147

Argonne National Laboratory
Atomic Spectroscopy Facility....148
4.5 MV Dynamitron Accelerator Facility....149
Premium Coal Sample Program....150
Pulse Radiolysis Facility....151
Brookhaven National Laboratory
National Synchrotron Light Source....152
Kansas State University
High Energy Atomic Physics Facility....154
Notre Dame Radiation Laboratory
Pulse Radiolysis Facility....156
Radiolysis-ESR Facility....157
Oak Ridge National Laboratory
EN-Tandem Facility....158
Sandia National Laboratories/Livermore
Combustion Research Facility....159

Topical Index....162
Institutional Index for Offsite Contracts....164
Investigator Index....169

Laboratory Project Data

All the summaries of projects funded by a particular Chemical Sciences program (e.g., chemical physics) in a particular Laboratory's division or department are in a contiguous sequence in this book. Total dollars for each such sequence are given at its beginning.

There are two numbers above each summary, other than its entry number. The number immediately to the right of the project title indicates the scientific person years devoted to the project. The other number is the four digit code which identifies the Chemical Sciences program which funds the project, as defined previously.

Photochemical and Radiation Sciences

Ames Laboratory — Total $290,000
Iowa State University
Ames, Iowa 50011

1. PHOTOPHYSICS, PHOTOCHEMISTRY AND SPECTROSCOPY — 2.7 — 01-01
G. J. Small

This project seeks an understanding of dressed excited states (polaritons) and ultra-fast coherent electronic energy transfer in molecular solids. It also considers photochemical, photoisomerization and photophysical processes of molecules in ordered and disordered solids utilizing coherent nonlinear laser spectroscopies to probe relaxation phenomena. Supersonic jet spectroscopy applied to charge-transfer excited states and vibronic interactions in molecules is also studied.

2. PICOSECOND SPECTROSCOPY AND REACTION DYNAMICS — 3.5 — 01-01
W. S. Struve

This work concerns kinetic studies of organic redox photoreactions of species attached to semiconductor surfaces using picosecond fluorescence, absorption, and photocurrent transients. Measurements of excited state processes of organic carbanions in solution are contrasted to their behavior on surfaces. Mechanisms of vibrational energy transfer of large molecules in solution and gas phase are determined as well as photodissociation processes.

Photochemical and Radiation Sciences

Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Total $3,900,000

3. PREPARATION OF ORGANISMS, PHOTOSYNTHETIC PIGMENTS, AND BIOLOGICAL MATERIALS OF UNUSUAL ISOTOPIC COMPOSITION — 0.7 — 01-01
H.L. Crespi, J.J. Katz, J.R. Norris, M. Wasielewski

This program has as its objective the production of photosynthetic microorganisms substituted with biologically important stable isotopes. The major effort is in the production of fully deuterated organisms, but in addition the ANL Chemistry Division is able to grow organisms in which non-magnetic ^{12}C is replaced by magnetic ^{13}C, ^{14}N by ^{15}N, ^{16}O by ^{17}O or ^{18}O, and ^{24}Mg by ^{25}Mg. Large quantities of green algae, blue-green algae, and photosynthetic bacteria are routinely available in unnatural isotopic composition involving either single or multiple substitution. These organisms, and the compounds obtainable from them, have important applications in magnetic resonance spectroscopies, small-angle neutron scattering, and resonance Raman spectroscopy. Of particular interest are applications in the study of chlorophyll, photosynthesis, biomimetic photochemistry, and bacteriorhodopsin.

4. GAS PHASE RADIATION CHEMISTRY RELEVANT TO COMBUSTION AND ATMOSPHERIC REACTIONS — 2.0 — 01-01
C. D. Jonah, W. A. Mulac

In this program, rate constants for simple free radical reactions are being measured, many of which are of great importance in atmospheric and combustion chemistry. The pulse radiolysis technique makes it possible to measure the kinetics at pressures of one atmosphere and above and over the temperature range of 50° to 1000°C, a range no other single experimental technique can easily span. The reaction rates of OH and OD radicals with CO and simple organic compounds are under investigation. In addition to the practical importance of these reactions to combustion, the data serve as an excellent test for reaction theories because of the rigorous restrictions provided by the wide temperature range and the use of two hydrogen isotopes.

5. CHLOROPHYLL AND PHOTOSYNTHESIS RESEARCH — 4.5 — 01-01
J. J. Katz, J. C. Hindman ,

The principal objective of this research is to acquire sufficient knowledge of chlorophyll function in natural photosynthesis to make possible ultimately the replication of the natural primary light conversion event outside the living cell. Current research focuses on: (a) laser photochemistry and photophysics of chlorophyll, with particular attention to new model systems; (b) energy transfer from highly excited chlorophyll a states; (c) new methods for the synthesis of chlorophyll model systems, including oxidative coupling at the C-10 position of Ring V; (d) applications of californium-252 plasma desorption mass spectroscopy to chlorophyll systems; and (e) structural studies by small angle neutron scattering of chlorophyll aggregates and natural photoreaction centers.

Chemistry Division, ANL, continued

6. ELECTRON TRANSFER PROCESSES AND ENERGY CONVERSION AND STORAGE STUDIED BY RADIATION AND PHOTOCHEMICAL TOOLS — 7.4 — 01-01
J.R. Miller, D. Meisel, C.D. Jonah, K.H. Schmidt, M.C. Thurnauer, W.A. Mulac

This program is directed at the fundamental understanding of electron transfer between molecules held apart at fixed distances and the study of chemical mechanisms involved in the conversion and storage of light energy. Electron transfer rates are measured by pulse radiolysis of solids or compounds containing two functional groups separated by rigid molecular spacers to determine the effects of distance, energy, and molecular structure. The work on energy conversion and storage utilizes various microenvironments (1) to enhance charge separation and thus the efficiency of photoelectron transfer, and (2) to increase the yield of photo-redox products while minimizing the rates of back reactions. Particular attention is given to mechanistic studies of catalytic water-splitting in colloidal systems and in microenvironments such as micelles, polyelectrolytes, and membranes.

7. PHOTOSYNTHESIS STUDIES: NATURAL AND ARTIFICIAL REACTION CENTER STRUCTURES AND MECHANISMS — 6.5 — 01-01
J. Norris, M. Wasielewski, M. Thurnauer, M. Bowman

The goal of this research is to elucidate in detail the utilization of light energy at the molecular level by natural photoreaction centers so that efficient artificial systems can be constructed. Emphasis is placed on the determination of the structural arrangement during the natural photosynthetic charge separation process for duplication in artificial photosynthesis. Very fast magnetic resonance techniques are used to measure distances, orientations and dynamics among the molecular components which participate in the transfer of electrons. Charge separation in single crystals of the reaction centers of photosynthetic bacteria also is being studied with magnetic and optical spectroscopy as well as x-ray and neutron diffraction.

Chemistry Division, ANL, continued

8. RADIATION CHEMISTRY AND PHOTOCHEMISTRY OF LIQUIDS AND SOLUTIONS — 14.6 — 01-01
A. D. Trifunac, C. D. Jonah, M.C. Sauer, Jr., S. Gordon, K. H. Schmidt, D. Meisel

The objective of this program is the study of chemical and physical processes that follow ionization (or photoionization) in both polar and nonpolar liquids. This is relevant to radiation chemistry, for the understanding of breakdown in dielectric liquids, and for the understanding of charge separation, recombination, and transfer, phenomena which are the basis of chemical and biological processes of energy storage and utilization. Various methods of radiation chemistry and photochemistry are used to provide details of the nature and dynamics of the early transient species and their chemical fates. This includes the study of electrons and positive ions, radical ions and excited states, and the subsequent fragmentation of the excited species into radicals and molecular species. Spin dynamics in radicals and radical ions is being used to provide better understanding of reaction kinetics. Essential tools used in this program are the Argonne high-current picosecond electron linac, the pulsed Van de Graaff accelerator, and innovative, time-resolved, magnetic resonance and laser techniques which are being developed and applied to these problems.

9. ARTIFICIAL PHOTOSYNTHESIS — 4.3 — 01-01
M. Wasielewski, J. R. Norris

The goal of artificial photosynthesis research is the development of molecular systems in the laboratory that not only mimic but improve upon natural photosynthetic energy conversion. This work focuses on several interrelated facets of this problem. First, a molecular design program involves the synthesis of molecular models of the natural energy conversion system. These models, through their mimicry of features of natural photosynthesis, aid in the structural and mechanistic understanding of the natural process. Second, the photophysics and photochemistry of these systems are studied with emphasis on light-induced electron transfer reactions. Advanced spectroscopic techniques such as picosecond spectroscopy and time-domain magnetic resonance are used to study these ultrafast processes. Third, the primary photosynthetic processes themselves are being investigated with a view toward integrating the information obtained from the laboratory systems with new knowledge of natural photosynthesis.

Photochemical and Radiation Sciences

Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973

Total $2,665,000

10. RADIATION CHEMISTRY — 11.2 — 01-01
B. H. J. Bielski, R. A. Holroyd, H. A. Schwarz

This program uses radiolysis and photolysis, emphasizing pulse methods, to study the behavior and reactions of transient chemical species (ions, electrons, free radicals, and excited states of molecules). Some experiments also involve the use of VUV radiation at the National Synchrotron Light Source. Principal areas of investigation are: properties and reactions of electrons in dielectric fluids, reactions of superoxide radicals and singlet oxygen, reactive metal ion intermediates in redox reactions, and electron transfer reactions in photosynthesis. The aims of the program are to provide the basic knowledge needed for the understanding and control of chemical reactions involving transient species, many of which are components of energy production processes (direct solar conversion, combustion, etc.) or are harmful consequences of these same processes (corrosion, environmental pollution, etc).

11. PHOTOCHEMICAL ENERGY CONVERSION AND SOLUTION KINETICS — 11.7 — 01-01
N. Sutin, C. Creutz, T. L. Netzel

Transition metal complexes strongly absorb visible light and readily undergo electron-transfer reactions. They are excellent mediators of outer-sphere light-induced redox reactions, many of which effect net storage of the light energy, and can also provide homogeneous catalytic routes for the thermal and photochemical formation of H_2 or the activation of CO. This program encompasses fundamental studies of the reactions of both excited-state and ground-state complexes. Since efficient light conversion and storage require the diversion of a significant fraction of the electronically excited molecules into "useful reactions" which must be driven in competition with rapid physical deactivation processes (luminescence and radiationless decay) and chemical "back-reactions", a major objective of this program is the quantitative study of these physical and chemical deactivation processes. In addition, because the overall efficiency of the conversion sequence may be limited by the rate of the subsequent "chemical" steps, mechanistic studies of the reactions of transition metal ions in high and low oxidation states are being conducted.

Chemistry Department, BNL, continued

12. ENERGY TRANSFER IN CHEMICAL KINETICS — 6.1 — 01-01
R. E. Weston

Chemical reaction rates depend strongly on the distribution of reactant energy among translational, rotational, vibrational, and electronic degrees of freedom. Conversely, the energy distribution in reaction products provides a sensitive probe of the reaction dynamics. Collisional energy transfer plays an important role in the reaction mechanism as a process by which energetic species are produced or removed. In this program, the transfer of translational, vibrational, or electronic energy is being studied. Atoms or molecules are produced in excited states by a pulse of ultraviolet, visible, or infrared radiation. The time-dependent disappearance of these excited species is monitored by the detection of radiation either from the parent species or from molecules that have been excited by collisional energy transfer. In a complementary part of this program, laser-induced reactions, including detailed studies of the laser energy absorption process, energy flow within excited molecules, and energy transfer from excited species, are being studied.

13. CHEMISTRY OF ENERGETIC AND UNSTABLE SPECIES: BASIC RESEARCH AND APPLICATIONS TO CHEMICAL CATALYSIS — 4.6 — 01-01
A. P. Wolf, R. A. Ferrieri

In part, this program investigates the basic chemistry of atomic and molecular species in neutral or charged states possessing electronic and translational excitation. Included are studies of the reactive intermediates produced by nuclear processes in the gas-phase and of the reaction pathways available to C, N, O and halogen atoms during atom-molecule encounters. New methods of atomic species generation will use synchrotron "light" to produce concentrations of molecular ions high enough to allow standard instrumental analysis of the final products. The development of a new type of electrostatic ion accelerator to produce intense beams of charged atoms and low molecular weight species will also be approached. A second effort of this program uses cyclotron-generated radionuclides in catalyst research, permitting studies to be performed at femtomol concentrations.

Photochemical and Radiation Sciences

Department of Applied Sciences
Brookhaven National Laboratory
Upton, New York 11973

Total $1,180,000

14. PORPHYRIN CHEMISTRY — 6.7 — 01-01
J. Fajer

This program addresses the function of chlorophylls in the photosynthetic transduction of light into chemical energy, the catalytic role of porphyrins in bioenergetic enzymic reactions, and the application of these reactions to synthetic multi-electron photocatalysts for the fixation of carbon and nitrogen, and the decomposition of water. The work encompasses synthetic, structural, physical and theoretical chemistry, and presently includes the storage and transfer pathways of oxidizing equivalents in peroxidases and photosystem II; the six-electron reduction of nitrite to ammonia mediated by isobacteriochlorins; theoretical and experimental modeling of environmental effects (ligands, charges, Schiff bases, conformations) on the properties of porphyrin and chlorophyll radicals; X-ray and neutron studies of Chlorobium chlorophylls as models for primary acceptors, and self-assembled aggregates of these chlorophylls as models of the light harvesting antenna of green and brown photosynthetic bacteria.

15. CONVERSION OF LIGHT BY SEMICONDUCTOR - ELECTROCHEMICAL SYSTEMS — 3.1 — 01-01
S. Feldberg and T. Skotheim

Two general areas of electrochemical research are being pursued: 1) Investigation of new materials which may be applicable to photoelectrochemical or electrochemical studies (e.g., electronically and ionically conducting polymers) and 2) Development of theory to analyze various photophenomena in semiconductors. Electronically conducting polymers (pyrroles, N-substituted pyrroles) are being examined using electrochemical and optical (FTIR, ESCA, EXAFS) techniques. A high vacuum electrochemical technique for the X-ray spectroscopy (ESCA and EXAFS) is being developed using a solvent-free solid polymer electrolyte (polyethylene oxide - PEO). PEO is also being investigated for use as electrolyte in a photoelectrochemical cell. Slow electron transfer between an electrode and a polymer-bound redox system appears to be a critical limitation. Computer modeling is providing a theoretical basis for the analysis of fluorescence decay in semiconductors following high intensity picosecond irradiation. Fluorescence quenching caused by surface modification (e.g., adsorbed benzoquinone or hydroquinone) can be characterized.

16. CHEMICAL PROPERTIES AND REACTIONS OF MONO- AND DINUCLEAR FERROCENE DERIVATIVES — 3.2 — 01-01
M. Hillman

This program is an investigation of the preparation and properties of metallocenes and related compounds that are expected to have application in the energy program, especially towards the splitting of water. Particularly, for the oxidation of water a bridged ferrocene was prepared and its reactions on a silicon electrode were studied. The oxidized state of the compound has a potential high enough to oxidize water and is stable under the alkaline conditions required; however, the electrode was not stable under these conditions. Compounds with higher oxidation potentials are required. For the reduction of water, the mechanism of the generation of hydrogen from [1.1]ferrocenophanes with strong acids is under study. Early results indicate that the release of hydrogen is the slow step. An understanding of this reaction will enable modifications of the compound so that hydrogen may be obtainable from weak acids, perhaps even water. Bridged ferrocenophanes were prepared. These compounds have tilted Cp rings and are expected to be protonated more easily than the parent non-bridged derivative and therefore to release hydrogen at a lower pH.

Department of Applied Sciences, BNL, continued

17. PHOTOLYSIS IN THE ADSORBED STATE — 1.2 — 01-01
J. W. Sutherland

The research program is directed towards understanding the modifying influence of the surface environment and the state of aggregation of a sorbate molecule on its photophysical and photochemical properties. The investigation into the photochemistry of polynuclear aromatic molecules adsorbed on porous glass continues; short-lived absorbing species, prompt and delayed fluorescence properties and absorption and excitation spectra are being studied as functions of surface coverage, light intensity and the presence of quenchers. Detailed studies have confirmed that molecular cations, but not carbonium ions, are readily produced at High light intensities by a two-photon process. The observation of a broad excimer-exciplex-like emission at very low surface coverages (e.g., 1 molecule of anthracene for 400,000 $Å^2$ of surface) implies that excited molecules are interacting strongly with specific sites on the surface or that the sorbate molecules are arranged in highly-ordered micro-aggregates.

National Synchrotron Light Source
Brookhaven National Laboratory
Upton, New York 11973

Total $3,800,000

18. NATIONAL SYNCHROTRON LIGHT SOURCE - OPERATIONS AND DEVELOPMENT — 40.4 — 01.01
J. McTague and A. van Steenbergen

The objective of this program is to support operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers operation and maintenance of the two NSLS electron storage rings and its associated injector combination of linear accelerator-booster synchrotron; operation and maintenance of the photon beam lines of the VUV and X-ray storage rings; and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings by means of new developments in high resolution photon optics, state-of-the-art monochromators, X-ray mirror systems, detectors, and so on. The NSLS storage rings will provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources. An extensive R&D program is necessary in order to optimize performance characteristics and also to develop new beam line instrumentation which will permit users to take full advantage of the unique research capabilities to be offered by this important new facility.

Photochemical and Radiation Sciences

Chemical Biodynamics Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $870,000

19. ARTIFICIAL PHOTOSYNTHESIS — 4.1 — 01-01
Melvin Calvin, J. W. Otvos

We are seeking to devise a synthetic system to accomplish a photoinduced electron transfer across phase boundaries, the way natural chloroplasts convert light into chemical energy. We have demonstrated the transfer of electrons across the lipid walls of vesicles. Other types of charged, single surfaces such as SiO_2 colloid have been found to increase the reaction yield when a primary reaction product is electrostatically repelled from the surface and prevented from back-reacting. We have shown that polymeric sulfonates can also produce this result. Presently we are focussed on the natural catalysts which will be required at both the oxidation and reduction ends. An iron-sulfur cluster has produced hydrogen electrochemically but not yet photochemically. A cobalt complex can be photochemically reduced to Co(I) and produce hydrogen. On the oxidation side the natural catalyst is a manganese compound of unknown structure. We have shown that a manganese porphyrin in a suitable microenvironment can be oxidized to Mn(IV) by a photosensitizer with the concomitant production of an intermediate reductant. Mn(IV) can be used to produce molecular oxygen, if desired.

20. PICOSECOND PHOTOCHEMISTRY — 1.8 — 01-01
J. H. Clark

Proton-transfer and electron-transfer reactions of electronically excited molecules form the basis for virtually all existing and proposed methods for the photochemical fixation of solar energy. In this research, the techniques of picosecond laser spectroscopy are used to directly monitor, in real time, the dynamics of these ultrafast processes. Such studies provide insight into the details of the mechanism and kinetics of these reactions at the molecular level. This work has shown that the naphthols and substituted naphthols provide prototypical systems in which the dynamics of excited-state proton-transfer are exquisitely sensitive to subtle chemical changes. The effects of solvent environment, intermolecular and intramolecular hydrogen bonding, molecular conformation, and reactant geometry are being studied with the aim of quantifying their role in excited-state proton-transfer processes. Picosecond time-resolved resonance Raman spectroscopy is being carried out on a number of electronically excited organometallic complexes to establish the changes in both geometrical and electronic structure which occur upon photoexcitation.

21. PHOTON CONVERSION — 4.1 — 01-01
G. C. Pimentel

This research investigates the chemistry and energy movement as it occurs on electronically excited hypersurfaces. Since both natural and artificial photosynthetic processes depend upon the chemistry of electronically excited molecules, these studies aid in the design of systems for chemical storage of photon energy. Cryogenic solids furnish particularly favorable environments for the study of light-initiated and reaction-initiated movement between and on electronic hypersurfaces. Reactants under study include $O_2(^1\Delta_g)$, Hg ($^3P_1$ and $^1P_1$), and HI ($^1\Delta$ and $X^3\Sigma^-$) with various unsaturated compounds. Energy storage using near infrared light, photochromism, and hypersurface mapping are goals. Temporal aspects of electronically excited transient intermediates are examined using nanosecond infrared spectroscopy.

Photochemical and Radiation Sciences

Materials and Molecular Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $420,000

22. PHOTOCHEMISTRY OF MATERIALS IN THE STRATOSPHERE
H. S. Johnston

5.0 01-01

This research is concerned with fundamental gas phase photochemistry, emphasizing chemical species that occur in the stratosphere. Laboratory studies are carried out to obtain optical cross-sections, quantum yields, and rate coefficients for molecules and reactions currently important toward interpreting atmospheric observations. Studies using laser flash photolysis and laser resonance absorption show that the primary products of N_2O_5 photolysis are $NO_2 + NO_3$, not $2NO_2 + O$ as had been previously reported. Chlorine atoms react slowly with nitric acid vapor and, surprisingly, do not form NO_3 + HCl as reaction products. Measurements of this ultraviolet cross section of molecular oxygen in the Herzberg continuum show it to be a function of temperature and about 30 percent lower at stratospheric temperature than at room temperature, which has been used in atmospheric models. This effect may turn out to explain the anomalously high intensity of ultraviolet radiation recently observed in sites in the middle stratosphere.

23. PHOTON-ASSISTED SURFACE REACTIONS, MATERIALS AND MECHANISMS
G. A. Somorjai

2.4 01-01

This project explores photocatalyzed chemical reactions that take place at the solid-vapor interface. These reactions include the photodissociation of water (H_2O) to produce hydrogen and oxygen, and the photon-assisted reactions of carbon dioxide (CO_2) and water to produce simple hydrocarbons (photosynthesis). The purpose of these studies is to explore the mechanism of photon-assisted surface reactions and then to establish the optimum conditions (of surface structure, composition, temperature and reactant mixture) to maximize the rate of production of the desired chemicals (hydrogen and/or hydrocarbons). The materials that are being used include iron oxides, silicates, and sulfides of rhenium and molybdenum.

11

Photochemical and Radiation Sciences

Notre Dame Radiation Laboratory
University of Notre Dame
Notre Dame, Indiana 46556

Total $2,650,000

24. THEORETICAL STUDIES ON REACTING SYSTEMS — 8.5 — 01-01
D.M. Chipman, J.J. Kozak

Quantum and statistical mechanics methods are being developed to interpret phenomena in radiation chemistry and photochemistry especially those involved in chemical-dynamic processes related to energy storage and transfer. A comprehensive statistical mechanical theory of photo- and radiation-induced redox reactions in organized molecular assemblies such as monolayers and micelles is being developed. These latter studies have considerable relevance to our understanding of experiments in which organizates may be applied in photochemical processes to effect the storage of solar energy. New quantum mechanical methods to perform and analyze electronic structure calculations on molecules and transient free radicals are being developed and used in conjunction with existing methods to study microscopic properties such as molecular structures, potential energy surfaces, reaction mechanisms, photochemical properties, intermolecular forces, electron-solvent interactions, spin density distributions and various spectroscopic parameters of molecules. Quantum dynamical aspects of the interaction of radiation with matter, specifically the temporal decay of excited states of two- and three-level atomic and molecular systems, are being studied using new analytical techniques.

25. ORGANIC PHOTOCHEMICAL PROCESSES — 8.0 — 01-01
P.K. Das,

Nanosecond laser flash photolysis experiments are being carried out to examine the role of intermediates (radicals, biradicals, singlet and triplet states, exciplexes and ion pairs) on the photochemical reactions of organic systems in solution. Included are studies of addition, fragmentation, hydrogen abstraction and electron transfer reactions, intermolecular energy transfer between quasi-isoenergatic triplets, intramolecular transfer in molecules containing two chromophores, electron exchange interactions with stable radicals, energy hopping along a polymeric chain and energy trapping in copolymers containing several types of chromophores. Model systems being investigated include phenyl substituted polyenes and polyynes containing heteroatoms, aromatic hydrocarbons and carbonyl compounds, small ring heterocyclic systems, stilbene analogues and polymers containing carbonyl groups. The studies on energy migration in polymers are particularly relevant to photosynthesis and to possibilities for enhancing the properties of polymers toward photodegradation or photostabilization. Programmatic emphasis is on obtaining mechanistic details of photochemically induced reactions.

26. INORGANIC PHOTOCHEMICAL STUDIES — 10.0 — 01-01
G. Ferraudi

The photochemical properties of coordination complexes of copper(II), rhodium(II) and rutherium(II) with macrocyclic ligands are being investigated. Conventional laser flash photolysis methods are used and supplemented by product analysis. A sequential biphotonic excitation technique is also being used for probing the time and energy relationships between long-lived excited states. In addition, pulse radiolytic experiments are used to provide spectroscopic and rate information on active intermediates, such as coordination complexes in unusual oxidation states. This research is carried out with compounds that exhibit either a direct or sensitized photochemical redox reactivity for excitation in the visible region of the spectrum and are, therefore, candidates for use in solar energy conversion. Two families of compounds are the main targets of these studies: the phthalocyanines and complexes with macrocyclic ligands possessing simple structures. Elucidation of general relationships between photoreactivity and the molecular structure of macrocycles is an essential goal of this project. Some of the mechanisms under study may be seen to exhibit potential application to photocatalytic systems.

Notre Dame Radiation Laboratory, continued

27. MICROWAVE STUDIES ON RADIATION CHEMICALLY PRODUCED INTERMEDIATES — 7.5 — 01-01
R.W. Fessenden

Electron spin resonance (ESR) spectroscopy is being used to study radical structures, radical reaction mechanisms and kinetics, and the nature of electron spin interactions in fluids. Continuous in situ radiolysis generates radicals for characterization of their geometric and electronic structures by means of the observed ESR hyperfine patterns. The identity of the radicals produced and any subsequent transformations observed provide information on reaction mechanisms. Time-resolved experiments on radicals produced by pulse radiolysis measure reaction rates for intramolecular rearrangements and bimolecular disappearance, as well as rates of bimolecular spin relaxation and the extent of signal enhancement by chemically induced dynamic electron spin polarization. The latter quantities taken together with reaction rates provide very detailed information on reaction mechanisms in liquids. Pulsed microwave experiments, including ones using saturation recovery and electron spin echo techniques, provide information on relaxation times in a more direct way. The spin echo method also allows improved time resolution for fast reaction rate measurements. Microwave methods are also used to study electron attachment processes in high pressure gases and liquids.

28. TIME RESOLVED STUDIES OF PHOTOLYTIC REACTIONS — 5.5 — 01-01
R.W. Fessenden

Time-resolved microwave absorption methods are applied to characterize the charge distribution in intermediates produced by laser excitation. Particular attention is being given to measuring the dipole moments, i.e. the degree of charge separation, in various radicals, excited states and exciplexes that are intermediates in photochemical processes. Parallel optical experiments employing two lasers, one to form and the second to photolyse the intermediate states, are also being carried out. Applications are directed toward characterizing the various absorption bands of the intermediates in terms of their photochemical activity. Optical absorption spectroscopy is used for diagnosis. Where dissociation is observed, studies of the recombination kinetics of the resultant fragments often provide rate data not directly available. Two-pulse experiments involving laser photolysis and pulse radiolysis are also used to investigate photochemical activity of radiation chemical intermediates and reactivity of photoexcited states with radicals. These investigations are complimented by both steady-state and time-resolved ESR studies of photolytically produced radicals.

29. THEORETICAL ASPECTS OF RADIATION CHEMISTRY — 3.0 — 01-01
K. Funabashi, A. Mozumder

These studies relate to the physical and chemical behavior of the electron in its various aspects and in different phases. Attention is focused on the development of a unified theoretical framework capable of describing the various physico-chemical properties of solvated electrons such as their optical absorption spectra and transport properties. Problems associated with thermalization of radiation produced electrons in both gases and liquids are addressed to elucidate the nature and properties of reactions at early times, especially as they apply to track effects. Contributions of secondary electrons to the reactions within heavy particle tracks are being examined. The thermalization studies are being extended to examination of the time evolution of the effective electron temperature in molecular gases based on experimentally available elastic and inelastic cross-sections. Conclusions from these various studies are important both to many aspects of radiation chemistry and to applications where ions are important in, for example, fluorescence detectors and solid-state devices.

Notre Dame Radiation Laboratory, continued

30. SPECTROSCOPY OF REACTION INTERMEDIATES — 7.5 — 01-01
J. Hardwick, G.N.R. Tripathi

Laser-excited fluorescence, long path absorption, and chemical luminescence spectroscopy are being used to conduct high resolution spectroscopic studies of small molecules, radicals and ions in the gas phase. High-lying rotational and vibrational levels of small molecules in their ground and excited electronic states are being studied through their infrared, visible, and ultraviolet spectra. Collisional transfer of energy in excited electronic states is being studied with rotational resolution in order to investigate in detail the important processes by which relaxation occurs during single collisions. Transfer of electronic energy from metastable rare gas atoms is being used to dissociate hydrocarbons in the gas phase, producing intense emission from excited electronic states of radicals and ions.

31. ELECTRON TRANSFER REACTIONS — 6.0 — 01-01
P. Neta,

Pulse radiolysis techniques are being used to characterize the kinetic properties of short lived transient species involved in electron transfer and redox reactions. Approaches developed in this laboratory provide methods for examining electron transfer equilibria and allow the determination of one-electron oxidation or reduction potentials for various types of organic radicals. Details of the oxidation and reduction of organic molecules by both organic and inorganic radicals are being examined. Additionally, time resolved studies are used to determine the reactivities of the intermediates following radiation initiated cleavage of both organic compounds and inorganic ions. Special attention is given to electron transfer reactions involving metalloporphyrins and chlorophylls, which are important in photosynthetic environments and also to intramolecular electron transfer within organic radicals and metal complexes. The ultimate aim of these various studies is to expand our understanding of reaction intermediates so as to be able to predict their role in radiation, photochemical and conventional chemical systems.

32. INFLUENCE OF ORDERED MOLECULAR ASSEMBLIES ON CHEMICAL PROCESSES — 8.0 — 01-01
L. K. Patterson

These studies are directed toward developing a better understanding of the relationships between structure in organized molecular assemblies and the influence these assemblies may exert on kinetic behavior in bulk phase, assembly pseudophase, or at interfacial boundaries. A variety of unique properties has been observed for systems in which such assemblies - micelles, vesicles, spread monolayers and liquid crystals - are formed. Such properties under study include compartmentalization of reaction into microregions with well defined boundaries, non-homogeneous distribution of reactants, surface orientation of reactant molecules, surface charge effects and reduction in dimensionality of the reactant phase. Alterations in rates and reaction mechanisms that are observed in such assemblies strongly suggest the possibility for kinetic control over a variety of photochemical and radiation chemical processes not possible in homogeneous solution. Principal attention is now directed toward studies in spread monolayers because these latter assemblies provide for significant control in the degree of organization which may be imposed on a reaction system. Preliminary investigations are now being carried out in liquid crystals which exhibit phases of varying organization.

Notre Dame Radiation Laboratory, continued

33. RADIATION CHEMISTRY DATA CENTER — 2.0 — 01-01
A.B. Ross, W.P. Helman, G. Hug, I. Carmichael

The Radiation Chemistry Data Center (RCDC) maintains and continuously updates a bibliographic data base on radiation chemistry and photochemistry and provides a variety of information services to the scientific community. Retrospective searches are carried out and bibliographies on specific topics are prepared and made widely available. A current-awareness publication, Biweekly List of Papers on Radiation Chemistry and Photochemistry is produced from the data base and distributed to subscribers. Experimental data for reaction intermediates produced by light or ionizing radiation are compiled from the published literature. Data are included for photochemical and photophysical processes in solution. The data are stored in computer-readable files and are readily available for correlation and reformatting in various ways. Critical reviews of these data are prepared for publication. A goal of this program is the development of a numeric data base of kinetic and spectroscopic properties of reaction intermediates which can be effectively used by many types of users. These bibliographic and numeric data bases are expected to be of increasing importance in the basic scientific study of chemical processes in irradiated systems and in technological applications such as solar energy utilization and photochemical effects on the environment.

34. RADIATION INDUCED REACTIONS — 13.0 — 01-01
R.H. Schuler, L.K. Patterson, G.N.R. Tripathi

A wide variety of chemical reactions induced by the absorption of ionizing radiation are being examined using the Laboratory's broad base of highly developed chemical and instrumental methods for examining intermediates both in time resolved studies and by analysis of ultimate products. Improvements in dosimetry and time resolution at the LINAC pulse radiolysis facility allow detailed optical and conductometric pulse radiolytic studies to be carried out at nsec and longer times. Recent introduction of laser resonance Raman techniques allow parallel studies of time resolved vibrational spectra of intermediates. Currently focus is on the molecular and electronic structure of oxygenated radicals present in electron transport processes. Radiation chemical studies are also being carried out at the Notre Dame Heavy Ion Facility to examine track effects in radiation chemical reactions induced by low Z ions having LET's of 1-100 ev/Angstrom. These studies are aimed at providing information on the importance of track structure in radiation chemical processes. These track studies are complemented by studies at very high intensities using a Febetron as a radiation source.

Photochemical and Radiation Sciences

Research Division
Solar Energy Research Institute
1617 Cole Boulevard
Golden, Colorado 80401

Total $450,000

35. PHOTOPHYSICS AND PHOTOCHEMISTRY OF PORPHYRINS AND MODEL SYSTEMS FOR ARTIFICIAL PHOTOSYNTHESIS
J. S. Connolly

0.7 01-01

This program is concerned with fundamental studies of energy- and electron-transfer processes of excited states in a variety of porphyrin-related systems. The focus is on the detailed photophysical properties of porphyrins and on light-induced electron transfer in synthetic models of photoreaction centers. The goal is to contribute to an improved understanding of the molecular properties required for efficient light-induced electron transfer in artificial photosynthesis. Laser flash photolysis and fluorescence studies are being carried out on covalently linked porphyrin-quinones and on their unlinked constituents to sort out the effects of photophysical properties, redox potentials, molecular geometry, temperature and solvent properties (dielectric constant, viscosity) on the kinetics and mechanism of light-induced electron transfer and subsequent charge stabilization.

36. BASIC PHOTOELECTROCHEMISTRY RESEARCH
A. J. Nozik, J. A. Turner, A. J. Frank,
B. A. Parkinson, J. Cooper

3.5 01-01

Basic research is being conducted in the following areas: hot carrier effects in photoelectrochemical systems; energetics, kinetics, and characterization studies of semiconductor-electrolyte interfaces; colloidal and particulate semiconductors; and conducting polymers on semiconductor materials. Hot carrier injection is being verified via both supra-band-edge redox chemistry and dye sensitization experiments. The kinetics of minority carrier transfer across the semiconductor interface is being established by means of transient photocurrent experiments. New techniques for characterizing photoelectrochemical systems, such as chronocoulometry and photocapacitance, are being developed. The utility of Mossbauer spectroscopy for studying semiconductor particles and colloidals is being demonstrated; kinetic data are being obtained for several particulate systems. The nature of catalytic deposits on both naked and polymer-coated semiconductor electrodes is being studied. New polymers and catalyst combinations are being investigated as approaches to the stabilization of semiconductor electrodes against photocorrosion.

Chemical Physics

Ames Laboratory
Iowa State University
Ames, Iowa 50011

Total $640,000

37. STATISTICAL MECHANICS OF GASEOUS SYSTEMS
D. K. Hoffman

01-02

Statistical mechanics are used to develop a kinetic theory of polyatomic and reactive gases, transport, relaxation, and reaction processes in polyatomic fluids. It utilizes classical and quantum mechanical scattering theory in the development of collision models for molecules with internal structure which bear on gas phase chemical reaction rates, the interaction of gas molecules with solid surfaces and surface distributions established under nonequilibrium conditions. The project includes an investigation of the effect of surface coverage on the nature of binding sites, an exploration of interactions between adsorbed surface species, a study of surface migration and cluster formation, and adsorbate effects on the catalytic properties of surfaces. These models for irreversible lattice processes can be tested with polymer and other (nonsurface) systems for which extensive empirical data is available.

38. ATOMIC, MOLECULAR AND FREE RADICALS: CROSSED BEAM KINETICS
C. Y. Ng

01-02

This project involves crossed molecular beam studies bearing on the kinetics of fundamental processes in combustion and low pressure pyrolysis of hydrocarbons. It also includes the molecular dynamics of excited atoms and molecules, ion/molecule reactions, and high resolution photoionization of molecules, clusters, and transient radicals. An important aspect of the work is to understand the role played by stable molecules, intermediate radicals, and ions in flames.

Ames Laboratory, continued

39. MOLECULAR THEORY BONDING 01-02
K. Ruedenberg

This research concerns a theoretical determination of molecular properties, geometric, electromagnetic and spectral, and in particular of energy changes during chemical reactions through quantum chemical calculations of molecular electronic structures. It includes predictions of reaction energies and activation energies for elusive intermediates and transition states. Analyses are made of electronic rearrangements along reaction paths and their energetic and kinetic implications. Fundamental developments in many-electron quantum mechanics including electron correlation are made in order to achieve chemical accuracy by practical methods for predicting reaction mechanisms. Development of quantitative interpretative concepts are emphasized which can be used by nontheorists to analyze reliably and anticipate intuitively ab initio predictions. Studies of oxidation-reduction and exchange reactions involving carbon, nitrogen, oxygen, hydrogen and silicon, in particular reactions occurring during combustion, in the atmosphere and during hydrogenations are used as a test of the basic concepts.

40. ION CHEMISTRY - MASS SPECTROMETRY 01-02
H. J. Svec, G. D. Flesch

This research involves the ion chemistry of inorganic, organometallic and organic compounds and ions and complementary neutral fragments produced by electron bombardment. The latter leads directly into the chemistry of highly excited molecules and free radicals. The results bear directly on the origin of aromatic heterocyclic hydrocarbons produced in the combustion of natural gas, oil, wood and coal under fuel rich conditions.

Chemical Physics

Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Total $1,680,000

41. HIGH RESOLUTION SPECTROSCOPY AND EXCITED-STATE DYNAMIC PROCESSES — 3.3 — 01-02
H.M. Crosswhite, F.S. Tomkins, K.T. Lu

The vacuum ultraviolet coherent-radiation facility, which makes use of nonlinear optical mixing in mercury vapor, is now available for use as a flexible excitation source for a variety of spectroscopic experiments. This is the most efficient upconversion process known, providing five-nanosecond pulses of the order of 10^{11} photons/pulse in the range 1150-1230 Å, with a resolving power of several million. Present experiments include energy-level structural and lifetime studies of simple molecular systems and fundamental diamagnetic experiments on atomic hydrogen. This facility is reinforced by two large spectrographs, both with resolving powers near one million, covering the wavelength range 1200-9000 Å, which are being used primarily as survey instruments for more detailed laser-based experiments.

42. THEORETICAL CHEMISTRY — 6.5 — 01-02
T. H. Dunning, Jr., M. J. Davis, L. B. Harding, R. L. Shepard, A. F. Wagner

This program is concentrated on theoretical studies of the energetics and kinetics of chemical reactions, with an emphasis on reactions of importance in the oxidation of hydrogen and simple hydrocarbon fuels. The basic thrust of the program is on the calculation of accurate molecular interaction potentials, the study of the chemical dynamics on the computed (or other realistic) potential energy surfaces, and the characterization of the molecular species (including ephemeral species) involved. In addition, there is a continuing effort devoted to the development of the theoretical and computational methodology needed to provide a realistic description of these fundamental chemical processes.

43. MOLECULAR BEAM AND METAL CLUSTER CHEMISTRY RESEARCH — 5.3 — 01-02
S. Wexler, E. K. Parks, S. J. Riley

The study of heterogeneous catalysis on a molecular level is being pursued. Beams of catalytically active naked metal (Ni, Cr, Ag, Cu, Al, Fe) atom clusters containing 2 to 20 atoms are generated either continuously or in pulses and their physical and chemical properties are characterized by laser based, in-flight diagnostic techniques. Spectral and electronic properties are determined and experimental results are correlated with theoretical calculations. Mechanisms and kinetics of adsorption and catalytic processes on surfaces of clusters are determined by the flow tube technique. The transient products are identified by laser ionization mass spectrometry.

19

Chemical Physics

Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973

Total $2,480,000

44. THEORETICAL CHEMISTRY — 7.2 — 01-02
S. Ehrenson, J. T. Muckerman, M. D. Newton

The goals of this program are to apply theoretical methods to the study of energy flow in chemical reactions and to the elucidation of molecular interactions involved in the storage and interconversion of energy in the gas phase and in condensed phases, including phenomena associated with charged species (i.e., solvation and charge-transfer processes). The methods principally used are ab initio and semiempirical calculations of the energies and structures of molecules in specific electronic states, and classical and semiclassical treatments of the nuclear motion in kinetic processes involving these systems. Many of the techniques currently being developed and applied in this program play an important role in analyzing and interpreting experimental data obtained in experimental programs in the Department.

45. ION-MOLECULE REACTIONS WITH APPLICATIONS TO FUSION ENERGY SYSTEMS — 5.8 — 01-02
L. Friedman, R. J. Beuhler

The development of high molecular weight mass spectrometric techniques has provided a facility for the investigation of nucleation processes responsible for the formation of cluster ions and neutral microclusters. Immediate goals are the development of cluster-ion sources and their exploitation as a basic research tool. A high molecular weight mass spectrometer which has the capability of mass analysis of molecular species with m/e values up to approximately 200,000 is now in use. Efforts to extend this mass range to higher m/e values are being pursued using high voltage ion post-acceleration, and with the development of time of flight mass analytical techniques. Ion source facilities capable of generation of plasmas from gases cooled to temperatures as low as 10 K will be used to study cluster ion generation from inert gases and diatomic molecular species. The generation of cluster ions from hydrogen isotopes is considered a major task objective because of the potential role these cluster ions may have in the study of controlled thermonuclear reactions.

46. GAS-PHASE PHOTOIONIZATION AND PHOTOELECTRON SPECTROSCOPY OF MOLECULES AND CLUSTERS — 3.9 — 01-02
J. R. Grover, M. White

Fundamental data necessary to understand fast, exothermic gas phase reactions are being measured via photoionization of molecular beams. This work utilizes tunable, monochromatic radiation from the recently completed gas-phase beamline on the VUV storage ring at the NSLS. Excitation function measurements on mass-selected ions are being carried out for van der Waals and hydrogen-bonded dimers and clusters, free radicals, and molecules. From these data heats of formation and binding energies are determined for both neutral and ionized product species, and studies are made of the Rydberg structure and dissociative ionization pathways of molecules and weakly-bound dimers from which an inner-valence electron has been excited or ejected. New experiments involving the use of electron energy analysis following the resonant, multiphoton excitation and ionization of small molecules, are also being performed. From the observed electronic and vibrational state distribution of the ion, it is possible to investigate in detail the electronic structure and ionization dynamics of electronically excited states of neutral molecules.

Chemistry Department, BNL, continued

47. CHEMICAL CRYSTALLOGRAPHY — 5.5 — 01-02
T. F. Koetzle, A. Kvick, R. K. McMullan

Neutron and x-ray diffraction methods are used to solve significant problems in crystal and molecular structure. Emphasis is placed on structures where hydrogen and other light atoms are important and on disordered or partially-ordered structures, since in these areas neutron diffraction, alone, or in combination with x-ray diffraction, has unique advantages for determining molecular structure and investigating chemical bonding. Completion of the chemical crystallography beamline at the National Synchrotron Light Source will open up new areas for x-ray diffraction studies. Examples of systems investigated under the crystallography program include organometallic compounds, transition-metal hydrides, zeolites, and pyroelectric and ferroelectric materials. Highly precise structures determined for simple molecules are compared to geometries derived from *ab initio* quantum mechanical calculations. Studies combining x-ray and neutron diffraction are also undertaken to examine electron charge-density distributions.

48. ELECTRONIC STRUCTURES OF SOLIDS AND THEIR SURFACES: STRUCTURE AND BONDING IN IONS IN SOLUTION — 4.5 — 01-02
T. K. Sham, R. Carr

The main objective of this effort is to improve the understanding of the electronic interactions among atoms in metals, alloys, metal oxides, and certain other compounds. It is especially important to learn about differences between the interactions in the bulk of such solids and interactions at the surfaces, and interaction of surfaces with adsorbates in order to study the heterogeneous physico-chemical phenomena at the interface. These studies are being carried out through photoelectron spectroscopy with conventional photon sources and synchrotron radiation at the NSLS. Studies are also being made of the geometrical and electronic structure of condensed matter, with emphasis on the systematics of the density of unoccupied states and the structure and dynamic behavior of metal complexes in solution. This work, an application of x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS), has been carried out during visits at the Stanford SSRL and will be pursued further at the NSLS. The results are directly related to certain kinetic and mechanistic aspects of chemical reactivity.

Chemical Physics

Department of Applied Sciences
Brookhaven National Laboratory
Upton, New York 11973

Total $420,000

49. KINETICS AND MECHANISMS OF ALTERNATIVE FUELS COMBUSTION
R. B. Klemm and J. V. Michael

5.2 01-02

The aims of this task are to make measurements of absolute rate constants for elementary combustion related reactions, and to investigate the mechanistic factors involved in gas phase combustion and pollutant formation processes. Emphasis is placed on alternative fuels that comprise a range of fuel types, including alcohols and hydrocarbon synfuels. To accomplish the aims of this task, a facility has been developed that features a wide variety of experimental techniques, including: flash photolysis-resonance fluorescence (FP-RF); discharge flow-resonance fluorescence (DF-RF); shock tube-atomic absorption (ST-AA); and discharge flow-photoionization mass spectrometry (DF-PIMS). The FP-RF and DF-RF methods are utilized in determining specific rates of elementary atom-molecule and radical-molecule reactions over a wide temperature span, ~200-1100K. The high temperature capabilities of this task have been extended to a considerable extent, up to ~2500K, by the recent addition of the shock tube apparatus. The DF-PIMS method is employed in this task to make direct observations of reactants and products for elementary reactions in an effort to investigate the relevant reaction mechanisms. This DF-PIMS experiment utilizes the National Synchrotron Light Source (NSLS).

Chemical Physics

Applied Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $96,000

50. UNIMOLECULAR KINETICS
M. Brown

1.25 01-02

Combustion chemistry consists of complex, multi-step chain mechanisms involving reactive radicals which are present in small concentrations. The complexity of the mechanisms, the inherent difficulties of working in high temperature environments, and the large number of species involved with the oxidation of an fuel make the study of combustion chemistry quite difficult. Our current research is concerned with the application of theoretical chemical kinetics to study unimolecular and bimolecular reactions important in combustion processes. The dynamics of reactions are investigated using classical trajectories with realistic potential energy surfaces. Special emphasis is placed upon elucidating the role of molecular angular momentum on intramolecular and intermolecular energy transfer and reactivity. Intermolecular energy transfer important in low pressure limit unimolecular kinetics has been investigated recently for prototype systems and compared with conventional models used to describe weak collision effects. Energy coupling effects have been elucidated. Research continues on microcanonical statistical theories and on diatom/diatom reaction dynamics.

Chemical Physics

Materials and Molecular Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $2,157,000

51. ENERGY TRANSFER AND STRUCTURAL STUDIES OF MOLECULES ON SURFACES — 2.6 — 01-02
C. B. Harris

This project is directed toward an understanding in a fundamental manner the way electronic excitation associated with the excited states of molecules is transferred to metal surfaces. The research utilizes short laser pulses to excite a molecule which is placed above an inert spacer gas at a specified distance above a metal crystal. The lifetime of the excited states is monitored by measuring the influence the metal surface has on the molecular emission. Utilizing this technique, it is possible to understand and confirm the theoretical basis for the processes down to a point where the molecule is only 10Å above a surface. Another part of this research is directed towards understanding in a fundamental way, the observation of surface enhanced photochemistry on noble metal surfaces. The photochemistry on silver shows a non-linear dependence on incident intensity, decreases sharply as the surface plasmon energy is approached, and is interpreted as enhanced multiphoton absorption due to enhanced surface electromagnetic fields at the silver surface, followed by fragmentation of the excited molecules out of photoionized states.

52. CROSSED MOLECULAR BEAMS — 8.0 — 01-02
Y. T. Lee

This research is directed toward the understanding of elementary atomic and molecular processes and primary photochemical processes using various molecular beam methods and laser facilities. In the area of dynamics of chemical reactions, the investigation of dynamic resonance phenomena in $F + H_2$, HD, and D_2 have been very successful. The crossed molecular beam studies of electronically excited Na atoms with HCl using a single frequency dye laser have also yielded some very interesting results. The reaction of $O(^3P)$ with acetylene was further investigated. It appears that the intersystem crossing from triplet to singlet plays an important role in the formation of $CH_2 + CO$ products. In the investigation of the primary photochemical processes of glyoxal, the prediction by Schaefer et al. of a concerted reaction forming $2CO + H_2$ was verified. In addition to the major channel producing $H_2CO + CO$, the formation of hydroxymethylene (CHOH) and CO was also observed. Other systems investigated include the $HD^v(v) + Na \rightarrow NaH^v + D$ and $NaD^v + H_2$ as a function of vibrational and translational energies.

53. MOLECULAR INTERACTIONS — 3.8 — 01-02
W. A. Lester, Jr.

This program is directed at extending fundamental knowledge of the dynamics of energy transfer, reactive, and photodissociative molecular processes. The approach is based on the reliable description of the potential energy surfaces and coupling matrix elements needed in theoretical approaches for the evaluation of cross sections and rates. Emphasis is placed on the use of state-of-the-art Hartree-Fock, multi-configuration self-consistent field and configuration interaction ab initio methods for molecular interactions, and various methods for collision dynamics. The electronic structure studies emphasize the determination of the critical geometries and energetics that govern reaction pathways and include the computation of global potential energy surfaces where appropriate. The dynamics studies involve ro-vibrational energy transfer in molecules by collision, and an adiabatic approach to chemical reaction and to single-photon photodissociation of small polyatomic molecules. A novel method that solves the Schroedinger equation stochastically is also being pursued to ascertain its usefulness for determining the energy and other properties of molecules.

Materials and Molecular Research Division, LBL, continued

54. THEORY OF ATOMIC AND MOLECULR COLLISION PROCESSES — 3.8 — 01-02
W. H. Miller

This research is primarily involved with the development of theoretical methods and models for describing atomic and molecular collision processes. The overall goal is to understand the dynamics of chemical phenomena at a molecular level and may thus be described as "molecular level chemical kinetics". Specific topics of interest include the theory of inelastic and reactive scattering, collision processes involving electronically excited atoms or molecules, collisional ionization phenomena, statistical theories of chemical reactions, scattering of atoms and molecules from surfaces, and the interactions of molecular systems with high power laser radiation. Much of this research is involved with the development and application of a general semiclassical mechanics that allows one to combine classical mechanics and quantum mechanics in a correct and useful manner. Certain research topics are more amenable to a completely quantum mechanical approach, and these sorts of theoretical techniques are also used.

55. SELECTIVE PHOTOCHEMISTRY — 3.0 — 01-02
C. B. Moore

Lasers are used to produce molecules in specific excited states. The ensuing chemical reaction and energy transfer processes are studied by spectroscopy and chemical analysis. Highly vibrationally excited molecules are produced by excitation of high overtones of single chemical bonds using visible lasers. The possibility of bond selective reaction is being studied in the gas-phase for cyclobutene and cyclopropylcyclobutene. Vibrationally specific photoionization of liquid water is being studied as a function of temperature. High overtone spectral structure is measured with a laser optoacoustic spectrometer to obtain information on transfer of vibrational energy among the modes of a molecule. The relative rates of chemical reaction and energy transfer determine the possibility of bond selective chemistry.

Chemical reaction rates of free radicals important in combustion are measured. A pulsed uv laser produces radicals and a cw dye laser monitors radical concentration as a function of time to give chemical reaction and energy transfer rates. CH_2 and CHO are now being studied.

56. PHYSICAL CHEMISTRY WITH EMPHASIS ON THERMODYNAMIC PROPERTIES — 2.5 — 01-02
K. S. Pitzer

The primary purpose of this program is the development of methods of prediction of thermodynamic properties of important and frequently complex systems. The relativistic quantum mechanical program for the calculation of dissociation energies and other properties of molecules containing very heavy atoms, recently developed in this project, is being applied to PtH, PtH^+, PbO, and PbH with calculations on SnO for comparison. Calculations are also in progress for UF_6, NpF_6, and PuF_6 in collaboration with LLNL. The methods are being modified and extended for calculations on larger clusters of atoms to investigate surface and catalytic properties.

Earlier work on the statistical thermodynamics of ionic systems is extended to the heat of unsymmetrical mixing. Good agreement is found with heat of mixing measurements on the aqueous systems NaCl-$BaCl_2$ and NaCl-Na_2SO_4. Statistical thermodynamic equations are being explored for the treatment of aqueous NaCl to 900 K and several kbar with the hope of prediction at even more extreme conditions.

Materials and Molecular Research Division, LBL, continued

57. SPECTROSCOPY AND STRUCTURES OF REACTIVE INTERMEDIATES — 2.5 — 01-02
R. J. Saykally

A variety of spectroscopic techniques are being developed for the purpose of detecting and characterizing reactive intermediates of importance in combustion processes. Far-infrared laser magnetic resonance (LMR) is being employed to measure rotational spectra of reactive intermediates with unpaired electrons. A new technique, called molecular beam laser electric resonance (MBLER), is being developed for the study of rotational spectra of polar species produced and cooled to extremely low temperatures in a supersonic expansion. Most recently, we have begun construction of a tunable far-infrared laser spectrometer which will compliment the preceding two experiments, carried out with fixed-frequency lasers, albeit with a somewhat reduced sensitivity.

58. POTENTIAL ENERGY SURFACES FOR CHEMICAL REACTIONS — 5.5 — 01-02
H. F. Schaefer, III

This research program has two purposes, related yet distinct. The first goal is the development of new theoretical and/or computational methods for the description of molecular electronic structure. Specifically, the single outstanding problem in the field is the correlation problem, that of formulating models for going beyond the single-particle or Hartree-Fock approximation. The second goal of this research is to apply these theoretical methods to significant problems of broad chemical interest. Currently, two areas of special interest are: (a) model theoretical studies of organometallic compounds, chemisorption, metal clusters and catalysis, and (b) the potential energy surfaces which govern gas-phase chemical reactions. Research in the former area is aimed at a truly molecular understanding of catalysis, a subject pertinent to future energy requirements, but sometimes approached by brute force trial and error methods.

59. PHOTOELECTRON SPECTROSCOPY
D. A. Shirley

This program addresses both experimental and theoretical aspects of electron spectroscopy for the investigation of electronic structure of matter in the gas and condensed phase. Research is conducted using both laboratory sources at LBL and synchrotron radiation in the energy range 5-5000 eV available at the Stanford Synchrotron Radiation Laboratory where there is participation in developing the spectroscopy of this newly-accessible range of the electromagnetic spectrum. Time-of-flight measurements with synchrotron radiation are used to measure angular distributions of photoelectrons and resonant photoemission phenomena in gas phase. Ultrahigh resolution photoelectron spectroscopy based on molecular beams is yielding new information about small molecules and about the transition from single metal atoms to behavior characteristic of a three-dimensional solid. Employing angle-resolved, variable energy photoemission and electron energy loss spectroscopy, this program examines the electronic structure of solids as well as geometric and electronic structure of surface-adsorbate systems with photoelectron diffraction, ARPEFS, and surface EXAFS.

Chemical Physics

Chemistry Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $510,000

60. MOLECULAR RESEARCH WITH ELECTRON SPECTROSCOPY — 2.5 — 01-02
T. A. Carlson, M. O. Krause, A. Fahlman

A basic study of the photoelectron dynamics of molecules and metal vapors is being undertaken through the use of angle-resolved photoelectron spectroscopy and synchrotron radiation. Phenomena receiving particular attention include: the Cooper minimum, shape resonances, autoionization, correlation satellites, and inter-channel coupling. Systematic studies are being pursued on halogen acids, halomethanes, metallic halides, and various metal vapors including Ag, Ga, Pb and some 3d transition metal elements. Supportive calculations using the multiple scattering Xα method are being performed and correlated with observed minima and maxima in the cross sections and angular distribution parameters. Improved computer handling of the experiment has allowed the introduction of constant-ionic-state techniques.

61. PHOTOCHEMICAL, PYROLYTIC AND REACTIVE INTERMEDIATES BY ELECTRON SPIN RESONANCE — 1.1 — 01-02
R. Livingston

Labile free radicals are observed at steady state concentration by ESR in circulating fluids at pressures up to 200 atm and temperatures to 700°C. Radicals are formed pyrolytically and photolytically with and without the use of added radical initiators such as peroxides. Work has centered largely on substances that are constituents of fuels and that are related to the production and combustion of organic fuels. A study has recently been completed on a chain reaction that occurs during the pyrolysis of benzyl ether. ESR observations have permitted measurement of kinetic parameters for important steps in the process. Chemical product assays have given additional information that correlates well with the kinetic parameters. New studies have been started on properties of allyl radical and radicals derived from iso-octane.

Chemical Physics

Combustion Sciences Department
Sandia National Laboratories/Livermore
Livermore, California 94550

Total $4,790,000

62. TURBULENT REACTING FLOW RESEARCH — 4.0 — 01-02
R. Dibble, R. Schefer, S. Johnston

This research is directed towards an increased understanding of the coupling between the chemical kinetic and turbulent transport processes occurring in chemically reacting flows. The long-term goal is to use this understanding to improve predictive capabilities for turbulent combustion. Multi-species Raman concentration and temperature measurements, combined with simultaneous velocity determinations, have been compared with model predictions to estimate the influence of chemical nonequilibrium on mean turbulent flame quantities. A new laboratory incorporating a vertical flame tunnel (and making use of the CRF facility dye laser) was assembled and made operational. A chemically reacting turbulent flow cooperative group comprised of participants from private industry, universities, and Sandia has been formed.

63. SOOT CHEMISTRY — 4.0 — 01-02
W. Flower, R. Schmieder, R. Perry,
M. Gusinow, S. Johnston, W. McLean

This research is aimed at understanding the roles of chemical precursors in soot formation. Hydrocarbon-oxygen reactions are studied in flat flames and in flow reactors, where special diagnostics provide critical information. Laser photolysis is used in a slow-flow reactor to produce radicals, and a cw, laser-induced fluorescence system has been implemented to probe the subsequent radical-molecule reactions. Radiolysis and radiocarbon tracer techniques are being employed to study hydrocarbon particulate formation and its relevance to soot formation. Light scattering techniques are used to observe soot formation in a flame, to measure particle diameter and number density, and to relate that information to a variety of experimental conditions.

64. CRF DIAGNOSTICS RESEARCH - ADVANCED METHODS — 3.0 — 01-02
J. Goldsmith, M. Koszykowski,
F. Tully

This program supports three broad areas of diagnostics research: development of new techniques for detecting trace species in combustion environments, research on advanced methods for kinetics studies, and theoretical studies in support of CRF projects. In the first area, atomic hydrogen has been observed in a flame using multiphoton optogalvanic spectroscopy, representing the first direct in-situ optical detection of this extremely important radical in a combustion environment. Atomic oxygen and NO are also being studied with this technique. Spatially resolved absorption methods are being developed for measuring other radicals in flames. Kinetics studies based on pulsed laser photolysis/quasi-cw ultraviolet laser induced fluorescence are in progress, and polyatomic free radical spectroscopy is concurrently being pursued. Theoretical techniques involving electronic structure and scattering calculations, as well as approximate chemical kinetic theories, are being applied to a variety of CRF projects, including high-resolution spectroscopy, modeling, and kinetics studies.

Combustion Sciences Department, Sandia-L, continued

65. COMBUSTION RESEARCH FACILITY OPERATIONS AND VISITING SCIENTIST SUPPORT — 12.0 — 01-02
M. Gusinow, D. Benthusen, R. Johnsen

This task supports all phases of Combustion Research Facility operations: operation of the central Facility lasers, operation and maintenance of the Facility VAX computer and networked minicomputers, operation of the computer terminals to the Sandia CRAY, staffing of the shop and chemistry laboratory, and maintenance of the safety and control system. This task also provides support for visiting scientists and for the transfer of technology developed and implemented at the Facility to others in the combustion community. Visitor support includes technician and engineering staff dedicated to the visitor's project, computer time, shop work, and purchases used directly by visitors or in support of them. The transfer of technology activity provides technical information to industry and university scientists through workshops on relevant topic short courses in specialized areas, and combustion-related meetings and seminars.

66. CRF CENTRAL LASER SYSTEMS — 3.0 — 01-02
C. Layne, R. Farrow, M. Gusinow

This project includes the continued development of existing CRF central lasers, and research in support of future major laser systems. The tunable dye laser, Diana, is operational, with performance levels which meet or exceed design specifications in all significant characteristics. Beam delivery and control throughout the Facility have been demonstrated. SNLL and visiting scientist experiments are now routinely using Diana. Possible system improvements include frequency doubling to obtain radiation from 240 to 370 nm, and mode-locking to obtain sub-nanosecond pulses. A new multipurpose laser system, Sirius, has been installed and remote CARS demonstrated. This new Facility laser system, when fully completed, will provide several sources of high peak power, ultra-high resolution radiation, thereby adding CARS (and other non-linear spectroscopic) capabilities to all of the CRF laboratories.

Combustion Sciences Department, Sandia/L, continued

67. FLAME CHEMISTRY - MODELING AND EXPERIMENT — 6.0 — 01-02
J. Miller, R. Cattolica, W. McLean, R. Mitchell, M. Smooke, R. Kee

The principal objective of this research is the development of comprehensive models for the chemical processes which govern flames. New numerical techniques have been implemented to provide fast and accurate methods for solving the one- and two-dimensional laminar flame equations, thereby facilitating comparisons with a wide range of experimental results. Laboratory studies emphasize the use of laser probes for measurement of radical and stable species concentration profiles in flames. Other techniques, including molecular beam-mass spectrometry, are also employed. In the past year comprehensive models for acetylene oxidation and ammonia oxidation were developed. Results provide favorable comparisons with a very large body of experimental data. Further experiments on lean and rich acetylene flames and on cyano-containing flames are now underway.

68. CRF DIAGNOSTICS RESEARCH - NONLINEAR PROCESSES — 3.0 — 01-02
R. Palmer, R. Farrow, L. Rahn

This research effort is directed toward developing nonlinear optical diagnostic techniques in support of Combustion Research Facility programs. New normalization techniques are being refined for coherent anti-Stokes Raman spectroscopy (CARS), a leading technique for time-resolved measurements of major species concentrations and temperatures. These new in-situ normalization schemes provide accurate corrections to fluctuating CARS signals in high-pressure environments, and have been implemented in a CRF internal combustion engine experiment. They are also being implemented in a laminar flat flame for use as a reference standard. High-resolution inverse Raman spectroscopic measurements are providing precise high-temperature N_2 and CO lineshape data. The vibrational Stark effect discovered earlier is being quantified in a crossed-beam infrared absorption experiment to provide spatially precise CO spectra from a laboratory flame.

Atomic Physics

Physics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Total $1,800.00

69. PHOTOIONIZATION MASS SPECTROMETRY, PHOTOELECTRON SPECTROSCOPY AND PHOTODISSOCIATION — 4.5 — 01-03
J. Berkowitz, B. Ruščic, R. Pandolfi, J. P. Greene

Fundamental processes in the photoionization of atoms and small molecules are studied at high photon resolution. For molecules, alternative decomposition modes are investigated, providing important thermochemical values, structural and dynamical information. Photoelectron spectroscopy is focussed on the more difficult high-temperature vapor species, and reveals their detailed electronic structure. A recently completed apparatus is intended for the direct study of the spectroscopy and dynamics of molecular-ion decomposition, by analyzing the decomposition products from interaction of UV-laser radiation with selected molecular ions.

70. ATOMIC SPECTROSCOPY WITH FAST BEAMS AT ANL — 4.4 — 01-03
H. G. Berry

Measurements of $2s\,^3P_1$-$2p\,^3P_{0,2}$ transition wavelengths in highly-stripped two-electron atoms are continuing at the Argonne Tandem-Linac with ions of titanium. A new linear position-sensitive detector is being developed to replace the grating exit slit. A program of experiments utilizing laser excitation of fast ion beams has begun. Na and He^+ autoionization electron spectra following collisions of 1-MeV He^+ ions on selectively-excited NaI, $3p\,^2P_{3/2}$ target atoms have been observed. This atomic state was populated by a cw dye laser at 50° to the incident ion beam axis. Several experiments involving ion beam resonant excitation by collinear laser beams are under construction. Optical polarization measurements have been made of the light emitted from excited states of hydrogen and hydrogen-like helium following perpendicular carbon-foil excitation of protons, H_2^+ and He^+, at energies of 50-100 keV and 0.7 to 1.7 MeV. Alignments of 100% for highly excited states have been observed.

71. THEORETICAL ATOMIC PHYSICS — 1.1 — 01-03
K. T. Cheng

The main objective of this program is to improve the understanding of the effect of relativity and electron correlations on atomic processes such as photoexcitations and photoionizations. The emphasis is to develop and apply advanced relativistic many-body techniques to the studies of these processes where both relativity and correlation effects are important. Current efforts include studies of the systematic trend of autoionization spectra for Ar-, Kr-, and Xe-like ions. In particular, there is interest in the dynamics of Rydberg series interactions which determine the change in resonance profiles along isoelectronic sequences. Studies are also being done on the absorption spectra of Pd- and Xe-like ions in the region of 4d-nf, nf transitions with a combination of the relativistic random-phase approximation and the term-dependent Hartree-Fock techniques. The purpose of this study is to gain better understanding of the 4f orbital-collapse phenomenon and its effect on the absorption spectra of rare-earth elements.

Physics Division, ANL, continued

72. HIGH-RESOLUTION LASER-rf SPECTROSCOPY WITH ATOMIC AND MOLECULAR BEAMS — 3.1 — 01-03
W.J. Childs, L. S. Goodman, V. Pfeufer

This program is directed toward a detailed understanding of interactions in atoms and small molecules. In the recent past the spin-rotation and hyperfine interactions of alkaline-earth monohalide radicals have been systematically studied and their dependence on vibrational, rotational, and isotopic effects elucidated. Efforts are now underway to extend the high-precision techniques to determine the electric dipole moments of these molecules. A similar program aimed at a systematic understanding of the hyperfine interaction throughout the 4f-shell of the rare-earth atoms is underway concurrently.

73. DISSOCIATION AND OTHER INTERACTIONS OF ENERGETIC MOLECULAR IONS IN SOLID AND GASEOUS TARGETS — 4.9 — 01-03
D. S. Gemmell, E. P. Kanter

Argonne's 4.5-MV Dynamitron accelerator is used to study the interactions of fast (MeV) molecular ions with matter. A unique feature of the apparatus is the exceptionally high resolution (0.005° and 300 eV) in angle and energy obtained in measuring dissociation fragments. The apparatus also permits the coincident detection of up to three dissociation fragments. The work has two main objectives: (a) a study of the interactions of fast charged particles with matter with emphasis on those aspects that take advantage of the unique features inherent in employing molecular-ion beams (e.g., the feature that each incident molecular ion forms a tight cluster of atomic ions that remain correlated in space and time as they penetrate the target) and (b) a study of the structures of the molecular ions that constitute the incident beams. Current attention is being focussed on the production of highly-excited Rydberg atoms formed in foil-excited ion beams.

74. ELECTRON SPECTROSCOPY WITH FAST MOLECULAR AND ATOMIC ION BEAMS — 4.0 — 01-03
D. Schneider, E. P. Kanter, H. Kudo,
P. Arcuni, W. Stöffler

This research project is directed toward the understanding of interaction of fast (meV) ion beams with solids and gases. Spectroscopy of secondary electrons is used to study dynamic excitation processes and to study highly-excited states in projectile and target atoms. Cross-section measurements, spectroscopic investigation with high energy resolution, and coincidence measurements are performed. Using field ionization techniques, the yield of Rydberg states formed in fast atomic (H^+,He^+) and molecular (H_2^+,HeH^+) ion beams is measured when merging from thin foil targets. The electronic deexcitation of excited fragment ions from molecular-ion impact is investigated and compared to the case of atomic-ion impact. Yield measurements are performed using solid targets (Si, Au) and H^- and He^- as projectiles. Additional measurements, under channeling conditions, should yield information regarding surface analysis. First experiments on a Na vapor target using fast ion beams in combination with laser excitation are performed.

Atomic Physics

Physics Department
Brookhaven National Laboratory
Upton, New York 11973

Total $240,000

75. ATOMIC PHYSICS RESEARCH — 3.1 — 01-03
E. W. Jones and B. M. Johnson

Beams from the Brookhaven Double Tandem Van de Graaff Facility are used to study various aspects of ion-atom and ion-electron collisions. Energies for negative ions cover the range from about 1 to 9 MeV. Beams of almost fully stripped elements up to iron can be produced with energies from several MeV to several hundred MeV when the tandems are operated in the accel-decel and 3-stage configurations. A lesser degree of ionization is obtained for heavier elements. Charge transfer and equilibrium charge states in ion-gas collisions are studied with negative ions and with positive ions produced by the tandem accel-decel method. Inner-shell vacancy processes are also studied with these beams. An effort to measure electron ionization and excitation cross sections in an electron-heavy ion crossed-beam experiment is now in progress. Work to study the excitation and ionization of atoms and ions by photons from the National Synchrotron Light Source has been started.

Materials and Molecular Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $473,000

76. ATOMIC PHYSICS — 6.0 — 01-03
R. Marrus

This research studies collision and spectroscopic properties of multi-charged ions. Measurements are made of cross-sections for electron capture by multi-charged neon ions on several rare gases. Using a novel trapping technique results are obtained at lower collision energies (Ne^{10+} at 1-10 ev) than have heretofore been possible. In another area, an experiment is being done to perfect observations of parity violation in atomic thallium. This effect represents a fundamental test of the new unified theories of electromagnetic and weak interactions. Using the highly stripped iron beam from the super-HILAC precision measurements are made on X-rays from hydrogenic and helium-like ions. These measurements exhibit effects due to quantum electrodynamics and relativistic effects. Dielectronic satellites associated with capture of an electron into a high-n state are also observed. These satellites are observed in fusion reactors where their intensities are used as a diagnostic tool.

Atomic Physics

Physics Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $1,130.00

77. THEORETICAL ATOMIC PHYSICS — 1.0 — 01-03
R. L. Becker and C. Bottcher

Theoretical predictions, interpretations of experimental results, and detailed calculations are made for atomic collision, radiation, and structure phenomena. Emphasis is placed on reactions of highly stripped ions and of electrons with atoms, particularly those reactions of importance in fusion energy devices and those studied in atomic high-energy accelerator physics laboratories. Recent activities include calculations of dielectronic recombination (being studied experimentally with merged beams at the ORNL EN-tandem Van de Graaff), multiple L-shell vacancy production by ions (being detected in x-ray satellites at the ORNL Holifield heavy ion accelerator), and ion-Rydberg atom collisions (for which the first experimental results, from the University of Kentucky, are appearing). New theoretical approaches include the "one and a half center" version of coupled-channels theory and the use of finite elements in the numerical integration of the time-dependent Schrödinger equation.

78. ACCELERATOR ATOMIC PHYSICS — 5.9 — 01-03
S. Datz, P. F. Dittner, P. D. Miller and C. D. Moak

The objective of this task is to achieve a detailed understanding of the interactions of high-energy, multiply-charged, heavy ions with gas, solid, and electron targets. The primary facility used is the EN-tandem accelerator. Ion-ion collisions at low energies are also being investigated, and two experimental programs have been started on the Holifield accelerators. Examples of subjects which have received particular attention during the past year are: 1) Cross section measurements of dielectronic recombination of B^{2+} and C^{3+} using a merged multiply charged ion beam concentric with an electron beam have been completed; 2) photodetachment and collisional detachment cross sections of He^- ions have been measured; 3) the study of radiation from channeled electrons and positrons has been continued; and 4) a program using positrons generated by the EN-tandem at all energies up to 6 MeV has been started. Results in these areas impinge directly on fusion research, solar corona studies, and material sciences, as well as improving our fundamental understanding of ion-atom, ion-solid, ion-ion, and ion-electron interactions.

79. EN TANDEM OPERATIONS — 1.6 — 01-03
P. D. Miller and G. F. Wells

The EN-tandem Van de Graaf is operated for atomic physics research. Terminal voltage up to 6.0 MV are achieved, and ions of all elements from Z=1 through 9 and many heavier ions are available for users. The user group includes members of the physics division, other divisions of ORNL, and faculty and students from various universities. During 1982 the design work for the installation of the Elbek Spectrometer was completed. The magnet was refurbished and long lead-time items were ordered. Sixty percent of the installation was completed. The major beam usage was for the merged electron heavy ion beams experiments, positron source development, and channeling studies. A small (<20%) portion of the available beam time was devoted to University of Tennessee and other university users.

Physics Division, ORNL, continued

80. COLLISIONS OF LOW ENERGY MULTIPLY CHARGED IONS — 1.4 — 01-03
R. A. Phaneuf and D. H. Crandall

This experimental program is aimed at improving our understanding of inelastic collision processes involving multiply charged ions at the lowest attainable collision energies. The current emphasis is on measurement of total cross sections for electron capture by highly stripped ions from hydrogen atoms at energies below 1 kev/amu. Toward this end, two different experimental approaches are being pursued. A pulsed-laser-produced plasma is utilized as a unique source of low-energy, highly-stripped ions which are directed through a calibrated thermal-dissociation atomic hydrogen gas target. Charge and energy analysis is effected by a time-of-flight technique. Total electron-capture cross sections have been measured recently for Al^{+q} ions ($2 < q < 10$) and Fe^{+q} ions ($3 < q < 14$) colliding with H and H_2 at energies in the range 10-100 eV/amu, and provide data for testing predicted ionic charge scalings at low energies. An ion-atom merged-beams apparatus is also being developed for studying such collisions at center-of-mass energies as low as 1 eV/amu, where theoretical predictions of increasing cross sections with decreasing energy remain untested.

Laser Research and Development Department — Total $150,000
Sandia Laboratories/Albuquerque
P. O. Box 5800
Albuquerque, New Mexico 87115

81. ATOMIC PROCESSES — 1.5 — 01-03
A. Owyoung, J. P. Hohlmer, A. V. Smith

This research is directed toward the study of collisional interaction and energy relaxation processes in atomic and molecular systems using laser-based excitation schemes. Using resonant multistep laser ionization techniques, we have measured rates of transfer between rotational states of NO due to collisions with rare gas atoms and NO molecules. These studies are being extended to other systems. In addition, similar methods are being applied to study electronic energy transfer between colliding molecules and orientational relaxation. By using appropriately polarized light, NO molecules in one rotational level can be oriented so their average angular momentum lies along one axis. The decay of the orientation or its transfer to other rotational states by collision processes are then probed by other polarized lasers. Other processes which may be investigated include collision induced vibration and electronic state changes and autoionization of NO.

Chemical Energy

Ames Laboratory
Iowa State University
Ames, Iowa 50011

Total $892,000

82. ORGANOMETALLIC COMPLEXES IN HOMOGENEOUS CATALYSIS
R. J. Angelici

2.2 02-01

The major thrusts of this research are to understand the role of organometallic ligands in transition-metal-catalyzed reactions and to seek new catalytic reactions which provide energy-efficient routes to useful chemicals. Of particular interest are reactions of ethylene oxide with CO ligands of metal carbonyl complexes. It has been demonstrated that CO ligands in complexes of Fe, Ru, Mn, and Re react with ethylene oxide to form dioxo-carbene complexes of those metals. This type of reaction is being examined for possible catalytic applications. Studies of thiophene complexes of transition metals have been initiated for the purpose of providing some understanding of the hydrodesulfurization of organic sulfur-containing compounds.

83. CHEMICAL KINETICS AND REACTIVITY OF TRANSITION METAL COMPLEXES
J. H. Espenson

4.5 02-01

Organometallic complexes such as $(H_2O)_5Cr\text{-}R^{2+}$, R-Co(dmgH)$_2$L, and R-Rh(dmgH)$_2$L are under active investigation, as are dinuclear compounds having a metal-metal bond. The research concerns the reactions which occur, and their kinetics and mechanisms, especially reactions in which the metal-carbon bond is formed or broken, or in which the organic group, R, reacts further. Novel displacements by free radicals are being investigated using techniques such as stopped-flow kinetics, product competition ratios, stereochemical labeling, and flash photolysis. Included are classes of compounds important in Fischer-Tropsch reactions, such as α-hydroxyalkyls. Studies of metal-carbon bond homolysis permit: (a) evaluation of thermodynamic bond dissociation energies, (b) resolution of the mechanism of homolytic cleavage vs. competing heterolysis, (c) examination of novel free radical displacement reactions, and (d) evaluation of the kinetic reactivity of aliphatic radicals. Conditions are being developed for the use of metal complexes to generate aliphatic radicals in solution in a controlled manner.

84. NUCLEAR MAGNETIC RESONANCE (NMR) STUDIES OF COALS, CATALYSTS, AND AMORPHOUS SEMICONDUCTORS
B. C. Gerstein

4.0 02-01

Solid state NMR is used to infer chemical functionality in coals and products of coal conversion, e.g. solid asphaltenes, and probe hydrogen, silicon and aluminum in zeolites used for conversion of methanol to ethylene. In addition, the morphology of proton containing regions in amorphous silicon-hydrogen alloys, and the types of SiH_x groups present in these materials are studied by solid state proton and silicon NMR utilizing a variety of experiments involving the proton and silicon spin dynamics.

Ames Laboratory, continued

85. SPECTROSCOPIC AND KINETIC CHARACTERIZATION OF METAL OXIDE AND SULFIDE CATALYSTS — 1.9 — 02-01
C. L. Schrader

The goal of this research is to develop a fundamental understanding of the solid state and surface chemistry of heterogeneous catalysts and the mechanisms of catalytic reactions. Metal oxide and sulfide catalysts for producing synthetic fuels or for hydrotreating coal-derived liquids are being investigated; catalysts for energy-efficient routes to chemicals are also important in this research. Spectroscopic techniques such as laser Raman spectroscopy and Fourier transform infrared spectroscopy provide characterization of the catalysts and adsorbed species. In situ experiments are being performed involving functioning catalysts: simultaneous spectroscopic and kinetic measurements can be performed at temperatures and pressures typical of industrial operating conditions. These techniques provide a direct method for relating structure and composition to catalytic activity, selectivity, and stability. The effects of defect structures, structural disorder, and nonstoichiometry are particularly important for the metal oxide and sulfide catalysts being examined. Adsorption and reaction studies are being performed using pulsed or steady-state fixed bed reactors.

86. HIGH-TEMPERATURE GAS-PHASE PYROLYSIS OF ORGANIC COMPOUNDS — 1.9 — 02-01
W. S. Trahanovsky

This research is directed toward an understanding of the fundamental thermal reactions of organic compounds, especially those that could be important in the pyrolysis of coal and coal-derived liquids. The work can be divided into three main categories: 1) determination of the major pyrolysis reactions of model compounds; 2) preparation and study of the physical and chemical properties of reactive compounds thought to be intermediates in pyrolysis reactions; 3) determination of the importance of surface-catalyzed reactions under various pyrolysis conditions. Most pyrolyses are carried out using the Flash Vacuum Pyrolysis technique. Much of the work concentrates on the study of pyrolysis reactions that are thought to involve quinodimethanes as intermediates, on the preparation and characterization of these and related species, and on the thermal reactions of these species and products derived from them. Specific compounds under study include tetralins, 2,3-dimethylene-2,3-dihydrofurans, the furan analogs of ortho-quinodimethanes, and benzocyclobutenes, the closed forms of ortho-quinodimethanes.

87. STUDY OF SOLID-GAS REACTIONS WHICH INVOLVE STRUCTURAL CHANGES IN THE SOLID — 1.0 — 02-01
D. L. Ulrichson, A. H. Pulsifer

The objective of this work is to understand and describe the behavior of the class of solid-gas reactions which exhibit either expansion or contraction of the solid during reaction. In the case of solid expansion, the increased volume of the solid product closes diffusion paths for the gaseous reactant and stops the reaction at less than total conversion. The reactionof sulfur dioxide with calcium oxide (used for removal of sulfur dioxide from boiler flue gas) is an example in which only about thirty percent of the calcium oxide reacts before the reaction stops. Previous models have concentrated on the effect of the reduced porosity which results from product expansion. Data from this project indicate that diffusion of reactant through the solid product layer is as important as pore reduction. Inconsistencies in published results for several solid-gas reactions can be explained by inclusion of this term. Current work emphasizes measurement of diffusion rates through the pores and through the solid product layer.

Chemical Energy

Chemical Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Total $450,000

88. FLUID CATALYSIS — 4.4 — 02-01
J. W. Rathke, M. J. Chen,
R. J. Klingler, J. J. Heiberger

This research attempts to determine reaction mechanisms and to find new catalysts for the conversion of small molecules (e.g., CO and CO_2) to specific desired products. Currently under investigation is a series of organometallic complexes which catalyze the reaction of CO with H_2O to form alcohols. This reaction occurs by a new mechanism which does not involve a prior water-gas shift pathway. Also studied are a general catalytic method for homologation of methanol to ethanol and a new catalytic pathway for hydrogen reduction of carbonate ion; the latter reaction being relevant to the utilization of inorganic carbon resources (e.g., CO_2). The mechanisms of these reactions are being investigated using a combination of high-pressure kinetic, tracer, spectroscopic (including multinuclear FT-NMR), thermochemical, synthetic, and theoretical (molecular orbital) methods.

Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Total $1,458,000

89. INORGANIC AND FLUORINE CHEMISTRY — 3.0 — 02-01
E. H. Appelman, L. J. Basile,
L. Stein

This program undertakes the preparation and characterization of novel inorganic oxidants and fluorinating agents. In addition to the physical and chemical characterization of these compounds, the program is devoted to the identification and exploitation of applications of these exotic materials to other areas of chemistry. A major current thrust is the application of hypofluorites, particularly the recently discovered fluoroxysulfate ion, SO_4F^-, as reagents in organic chemistry, with especial emphasis on their use as selective fluorinating agents for biologically important steroids. Other current efforts involve elucidation of the mechanism of interaction of F_2 with aqueous solutions and the use of powerful fluorinating agents to prepare unusual, highly oxidized compounds of the actinide elements.

Chemistry Division, ANL, continued

90. THE PREMIUM COAL SAMPLE PROGRAM — 2.9 — 02-01

K. S. Vorres

The objective of this program is to provide the U. S. basic coal science research community with long-term supplies of a small number of premium coal samples. The premium coal samples produced and distributed by this program are to be as chemically and physically identical as possible, have well-characterized chemical and physical properties, and be stable over long periods of time. Coals are to be mined, transported, processed into desired particle and sample sizes, and packaged in environments which are as free of oxygen as possible and which maintain the natural moisture content to insure that the coals are kept in as pristine and stable condition as possible. These premium samples are to be distributed to researchers upon request. It is anticipated a computer data base will be included in this program to provide researchers with easy access to detailed information on sample availability, the physical and chemical properties of the coals, and references to the results of research obtained using these samples.

91. FUNDAMENTAL CHEMISTRY OF COALS AND OTHER FOSSIL FUELS — 6.5 — 02-01

R. E. Winans, R. Hayatsu, R. E. Botto, R. G. Scott, R. M. McBeth

The major objective of this program is to provide a fundamental understanding of the macromolecular structure of coals and coal macerals and to relate these structures to the chemical and thermal reactivity of these materials. Information gained in this study is important for improving current conversion processes and for designing new, novel processes. The approach taken in this study is to solublize selectively the macromolecules and to characterize the products by mass spectrometry, both solution and solid C-13 nuclear magnetic resonance, Fourier transform infra-red spectroscopy, and with a large variety of separation techniques. A chemically realistic model and new insight into the formation of coal macerals are resulting from these studies on artificial coalification. The characterization and reactivity studies of separated macerals are being emphasized. Correlations of these data by statistical analysis are providing additional insight into the structure-reactivity relationship of coal macerals.

Chemical Energy

Bartlesville Energy Technology Center
P. O. Box 1398
Bartlesville, Oklahoma 74003

Total $170,000

92. THERMODYNAMIC CHARACTERIZATION OF CONDENSED-RING COMPOUNDS — 3.0 — 02-01

B. E. Gammon

Research continues on synthesis, purification and measurement of thermodynamic properties of polycyclic aromatic hydrocarbons and their hydrogenation products and for similar polycyclic, organic, nitrogen compounds. These substances are important in processing of coal, oil shale, and heavy petroleum to produce liquid fuels and chemical feedstocks. Preparation of manuscripts is in progress reporting thermodynamic properties of 2,2'-dimethylbiphenyl, 3-methylpyrrolidine and isoquinoline. Measurements are nearing completion on quinoline, 4-methylphenanthrene and 2,6-dimethylpyridine; several other compounds are purified awaiting measurements. Synthesis and purification of others are in progress. Derived Gibbs energies of formation facilitate an understanding of hydrocracking and denitrogenation. The data also form the base for improved correlations based on molecular structure. The comprehensive experimental program involves enthalpy of combustion, low-temperature adiabatic calorimetry (third-law entropy determinations), PVT relations including vapor pressure, Raman and infrared spectroscopy and molecular statistical mechanics.

Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973

Total $400,000

93. ORGANOMETALLICS IN HOMOGENEOUS CATALYSIS — 2.9 — 02-01
M. A. Andrews

The efficient production of chemicals from coal and petroleum-derived feed stocks is increasingly dependent on homogeneous catalysts. Basic research in this area provides a foundation for rational catalyst design and improvement. Work in this laboratory is devoted to understanding the role of soluble transition metal complexes in the homogeneous catalytic oxidation of organic substrates. The long range goal of this work is the development of a more efficient, selective alkene epoxidation catalyst. A new approach to this problem employs transition metal nitro-nitrosyl redox catalysts to oxidise a wide variety of alkenes, with concurrent formation of the nitrosyl complex. The nitrosyl group is air oxidizable back to a nitro functionality, completing a catalytic cycle. The oxidized organic products produced and the selectivities obtained are strongly dependent on the type of alkene. A mechanistic understanding of these distributions has been obtained, and future studies will utilize the insights obtained to understand related existing catalyst systems and to develop new and more selective epoxidation catalysts.

94. MECHANISMS OF PHOTO-, ENZYME-, AND CHEMICALLY CATALYZED CIS-TRANS ISOMERIZATION — 2.9 — 02-01
S. Seltzer

Cis-trans isomerization can be brought about by the application of heat or light, or by catalysts. Because the physical and chemical properties of the two isomers differ, relaxation of a nonthermodynamic mixture of isomers (achieved by irradiation) to the thermodynamic mixture can result in the release of thermal or electrical energy. This cis-trans energy producing effect is utilized in biological processes, such as vision in animals and the light-driven proton pump of Halobacteria, which can be utilized in a photogalvanic cell. Studies at BNL are concerned with the mechanisms of enzymatically and chemically catalyzed and photosensitized cis-trans isomerizations and their application to the mechanisms of the proton pump.

Chemical Energy

Department of Applied Sciences
Brookhaven National Laboratory
Upton, New York 11973

Total $565,000

95. HIGH TEMPERATURE CHEMISTRY — 2.2 — 02-01
J. J. Egan

This is a study of the thermodynamic and transport properties of inorganic substances at high temperatures and attempts to explain the results in terms of appropriate atomic models. The substances include solid and liquid compound semiconductors, solid electrolytes, and molten salts. Electrochemical techniques are used to investigate the effect of composition on the concentration, mobility, and diffusion of electrons and electron holes in these substances. Cells employing solid electrolytes at high temperatures as well as molten salt electrolytes prove especially useful for characterizing these systems. High temperature calorimetry is being used to study liquid semiconductors and other liquid alloy systems. Molten salts are studied since they are important for the development of high energy-density batteries and fuel cells. The electronic conductivity of these melts in particular is examined by special techniques. Solid compound semiconductors of potential use as solar cells are studied by high temperature electrochemical techniques.

96. METAL HYDRIDES — 4.6 — 02-01
J. J. Reilly

The overall concern of this program is the determination of the thermodynamic properties and structural parameters of metal alloy-hydrogen systems. Particular goals are to relate the hydriding properties of metal alloys to their structure and composition, the determination of alloy-hydrogen phase diagrams, the determination and systematization of crystal structure and, finally, to relate all pertinent data and observations to develop a predictive capability regarding the behavior of a given alloy-hydrogen system. Current topics of interest are the causes of the observed deviations from ideal behavior of certain intermetallic-hydrogen systems, surface and near surface properties of metal-hydrogen systems, the partial molar volume of hydrogen in intermetallic compounds, the influence of defects upon system behavior and reaction kinetics of metal hydride suspensions. The major experimental tools and/or techniques consist of X-ray and neutron diffraction, equilibrium pressure-temperature-composition measurements, ion beam analysis and magnetic susceptibility measurements.

Applied Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $120,000

97. BIOCONVERSION OF CELLULOSE — 2.0 — 02-01
C. R. Wilke and H. W. Blanch

This project investigates primarily the enzymatic hydrolysis of biomass to hexose and pentose sugars. Basic information on the kinetics and mechanism of enzymatic hydrolysis is to be obtained. This information can then be used to develop low-cost processing schemes for sugar production. High productivity fermentations to convert these sugars to ethanol or other chemical feedstocks are being developed. Fundamental studies on yeast metabolism in high cell density cultures will be obtained. This will be combined with basic studies on ethanol separation from the fermentation broth, using novel, low-energy solvent extraction schemes.

Chemical Energy

Materials and Molecular Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $1,250,000

98. HIGH-ENERGY OXIDIZERS AND DELOCALIZED-ELECTRON SOLIDS.
N. Bartlett

5.0 02-01

The central concern of this program is in synthesis of new materials. The synthetic work exploits and tests theoretical models developed to account for the dependence of observed properties (such as electrical conductivity) upon chemical composition and structure. Present emphasis is on the study of two-dimensional extended atomic networks such as those derived from graphite, layer-form boron nitride and their relatives. Electron-oxidation of such materials (with salt formation) generates durable and conductive materials (some better than aluminum). Chemical, stoichiometric and structural requirements for the best conductivity are being defined. Some may have application as electrodes in electrochemical generation of potent new oxidizers. Recent findings indicate that fluorine can be intercalated, reversibly, into graphite by electrochemical means to a composition $\simeq C_{1.5}F$. Salts which are either proton or fluoride ion conductors, but not metallic, and which are resistant to oxidation, are being sought as solid electrolytes for use with the metallic layer-material salts.

99. TRANSITION METAL CATALYZED CONVERSION OF CO, NO, H_2 AND ORGANIC MOLECULES TO FUELS AND PETROCHEMICALS
R. G. Bergman

2.6 02-01

The goal of this project is the discovery of new chemical reactions in which transition metals interact with organic materials, and the understanding of how these reactions work. The approach begins with the synthesis and structural characterization of new types of stable organotransition metal complexes. Following that the self-reactions of these materials (induced, for example, by heat or light) are investigated, as well as their reactions with small molecules and organic compounds. A recent discovery on this project was the finding that a certain class of iridium complexes undergo oxidative addition into the carbon-hydrogen bonds of completely saturated hydrocarbons. This is the first example of this long-sought reaction, and work on this project is now directed at examining the scope, selectivity, and mechanism of this reaction. Efforts are also being directed at converting the alkyl(hydrido)iridium products of the oxidative addition into functionalized organic molecules.

100. FORMATION OF OXYACIDS OF SULFUR FROM SO_2
R. E. Connick

2.3 02-01

Sulfur dioxide is an atmospheric pollutant produced primarily from the burning of coal. The present research is aimed at a fundamental investigation of its chemistry and that of species formed from it so that processes for its abatement will be understood better and can be improved. The lability of the oxygens of HSO_3^- in aqueous solution is under study using the nuclear magnetic resonance of oxygen -17 as a probe. The results of the research should clarify the mechanism and rate of exchange of oxygen atoms between HSO_3^-, $S_2O_5^{2-}$ and H_2O. The rate of oxidation of HSO_3^- by oxygen is being investigated by following the reaction in the liquid phase with an oxygen meter. Because the reaction occurs by a chain mechanism, it is highly sensitive to impurities. The approach used is to add deliberately species that will control the initiation, propagation and termination steps of the chain so as to overwhelm impurity effects.

Materials and Molecular Research Division, LBL, continued

101. CHEMISTRY AND MORPHOLOGY OF COAL LIQUEFACTION — 1.5 — 02-01
H. Heinemann

This research is concerned with a better understanding of technologically important reactions, and potentially leads to new process applications. It has been found that hydrocarbons as high as C_6 can be produced directly from graphite and water at temperatures as low as 500°C and in the presence of alkali catalysts. Gasification and synthesis steps may thus be combined in a single operation. Mechanisms have been investigated. A selective hydrogenation of polynuclear aromatics containing nitrogen has been demonstrated with total selectivity for the nitrogen containing ring only.

102. SYNTHETIC AND PHYSICAL CHEMISTRY — 1.7 — 02-01
W. L. Jolly

In this research, ionization potentials from core and valence photoelectron spectroscopy are used to characterize the bonding in organometallic compounds related to catalytic systems. Most of this work involves the study of molecular compounds in the gas phase using x-ray photoelectron spectroscopy. Studies of the interactions of olefins and isocyanides with transition metals in complexes such as $LFe(CO)_4$ and $LCr(CO)_5$ yield detailed information about the σ- and π-bonding in such systems. The heats of formation of gaseous ions are obtained from the core binding energies. It is planned to use a high-temperature sample cell on the spectrometer to allow the study of compounds which have too low a vapor pressure at room temperature.

103. SURFACE CHEMISTRY - APPLICATION OF COORDINATION PRINCIPLES — 2.1 — 02-01
E. L. Muetterties

Establishment of the coordination chemistry of nickel and platinum surfaces represents the major thrust of this research. Definition of chemisorption states for important representative molecules from major classes of organic molecules and examination of catalytic reactions will comprise the major research objectives. Key organic molecules under investigation include thiophene, pyrrole, furan and aromatic hydrocarbons. In addition, these surface states will be modeled with molecular cluster complexes. Isotopically labeled cluster molecules such as $^{101}Ru_3(CO)_{12}$ and $^{104}Ru_3(CO)_{12}$ have been prepared for tests of metal-metal bond scission reactions.

Materials and Molecular Research Division, LBL, continued

104. ELECTROCHEMICAL SYSTEMS
J. Newman

0.7 02-01

This program includes investigation of fluid flow and electrochemical transport, analysis of mass-transfer rates and current distribution, design of practical electrochemical systems, and investigation of corrosion processes. Coupled kinetic, mass-transfer, and fluid-flow phenomena are investigated in semiconductor electrode systems, with emphasis on the optimization of configurational and operating parameters of liquid-junction photovoltaic cells.

6.5 02-01

105. CATALYTIC HYDROGENATION OF CO:
Catalysis on Well-Characterized Surfaces
G. A. Somorjai
Catalysis by Supported Metals
A. T. Bell

This research is aimed at developing a fundamental understanding of the chemical processes occurring during the hydrogenation of CO to hydrocarbons and oxygenated products. The experimental work involves measurements of reaction kinetics, elucidation of reaction pathways, and characterization of the catalyst surface using a variety of spectroscopic techniques. The influence of promoting Fe and Re with alkali metals, on the C_2^+ selectivity of these catalysts is being explored. High surface area thoria catalysts are being investigated for the synthesis of methanol. A study is being carried out of the structure and reactivity of different forms of carbon deposited on the surface of Ru during hydrocarbon synthesis. Attempts are being made to identify the physical and chemical interactions between Pd and metal oxide supports, which influence the performance of the Pd for methanol synthesis.

2.4 02-01

106. ORGANOMETALLIC CHEMISTRY OF COAL CONVERSION
K. P. C. Vollhardt

The basic program objective is to apply organometallic processes and techniques to the solution of problems concerned with the conversion of coal to liquid and gaseous fuels. Specific ligands to transition metal organometallic complexes are being constructed, the steric and electronic features of which have lead to the uncovery of novel processes in the coordination sphere of metals. Several of these constitute novel organometallic photochemical energy storage cycles. The use of light in the activation of complexed small ligands, such as carbon monoxide and carbon dioxide, is being explored. Morever, investigations are being carried out concerned with the activation of carbon-hydrogen and carbon-carbon bonds in coal model systems. Several novel molybdenum clusters have been prepared and their chemistry with respect to hydrodesulfurization is being studied. The reaction of sulfur with homogeneous transition metal clusters is being scrutinized as a potential analog to reactions occurring on catalytic surfaces poisoned by sulfur.

Chemical Energy

Chemical Engineering Division
Lawrence Livermore National Laboratory
University of California
P. O. Box 808
Livermore, California 94550

Total $184,000

107. EFFECTS OF METAL SURFACES ON KINETICS OF HYDRIDE FORMATION — 1.9 — 02-01
S. A. Steward

The objective of this study is to elucidate the surface chemistry of metals, alloys, and especially intermetallic compounds that react extensively with hydrogen. Many of these compounds are potential hydrogenation catalysts as well as hydrogen storage media. Important compounds, such as FeTi and $LaNi_5$, are being examined with a variety of modern surface techniques, such as Auger Electron Spectroscopy (AES), Low Energy Electron Diffraction (LEED), Secondary Ion Mass Spectrometry (SIMS), and Electron Stimulated Desorption (ESD). Our emphasis is now on single crystals of intermetallics, which should provide valuable insight into the gas adsorption mechanisms that affect hydrogen reactivity in the technologically important polycrystalline materials.

Chemistry Division
Los Alamos National Laboratory
University of California
P. O. Box 1663
Los Alamos, New Mexico 87545

Total $250,000

108. SYNTHESIS OF THERMOCHEMICAL CYCLES — 1.4 — 02-01
W. Jones, E. Onstott,
M. Bowman (Consultant)

This research is directed to an understanding of the basic chemistry and engineering principles required to synthesize efficient thermochemical cycles for the production of hydrogen from water by the use of heat sources such as solar, nuclear fission and nuclear fusion reactors. A general objective is to establish the criteria required for the development of this new technology and for the evaluation of worldwide programs. The research consists of the identification, initial evaluation, and preliminary development of different cycles through measurements of reaction rates, reaction yields, and thermochemical properties. Current studies include: 1) thermochemical and hybrid thermochemical-electrochemical cycles based on solid sulfate decomposition reactions, 2) low temperature reactions in cycles based on oxide decompositions, and 3) evaluation of key reactions in methanol-based cycles.

Chemical Energy

INC Division
Los Alamos National Laboratory
University of California
P. O. Box 1663
Los Alamos, New Mexico 87545

Total $225,000

109. LABILE SO_2 COMPLEXES — 1.25 — 02-01

C. J. Kubas, G. D. Jarvinen,
R. R. Ryan

The basic chemistry of sulfur dioxide is being expanded with regard to its binding to transition metal complexes, enhancing its reactivity, and promoting catalytic reactions. The ultimate goal is development of new methods for scavenging SO_2 from flue-gases. Work includes synthesis and structural characterization of new SO_2 complexes and catalytic reactions of SO_2 with other small molecules. For example, SO_2 and NO have been converted to sulfur, nitrogen, and water by hydrogen reduction over a Ru/alumina catalyst and methods of catalyzing such reactions homogeneously are being investigated. Reactions of SO_2 with transition metal hydride complexes are being studied in order to identify intermediates and mechanisms involved in hydrogen transfer to SO_2, and insertion of SO_2 into a metal-hydride bond, a possible key step in hydrogenation, has been observed for the first time. As a spinoff of the above work, the first example of a molecular hydrogen complex, $W(CO)_3(PR_3)_2(\eta^2\text{-}H_2)$, has been discovered, and its possible role in catalytic hydrogenation is under investigation.

Mound Facility
P. O. Box 32
Miamisburg, Ohio 45342

Total $233,000

110. FUNDAMENTAL INVESTIGATIONS OF METAL HYDRIDES — 2.5 — 02-01

R. C. Bowman, Jr., G. C. Abell,
M. P. Guse

The program objective is to obtain a fundamental understanding of the role of the interstitial hydrogen on the electronic and structural properties of the host metal. Experimental techniques such as NMR, variable temperature x-ray diffraction and thermal analysis are being used: 1) to evaluate specific properties of the electronic structure; 2) to determine the effect of host metal structure, hydrogen site occupancy, and alloy substitution on hydrogen diffusion; 3) to study the ramification of phase transitions on the electronic structure of the metal hydrides. Among the hydrides under current investigation are the AB_5 compounds, zirconium and titanium based alloys both crystalline and amorphous, and the Laves alloys. Monte Carlo type calculations are used to correlate NMR lineshapes with hydrogen site occupancy. Quantum-mechanical calculations of the electronic properties of clusters of metal atoms with hydrogen interstitials are being used to describe additional experimental results. Short range electronic structures are being explained using a localized electronics states model.

Chemical Energy

Chemical Technology Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $250,000

111. KINETICS OF ENZYME-CATALYZED REACTIONS — 3.1 — 02-01
E. Greenbaum, J. Woodward

This research is focused on understanding the fundamental chemical and physical mechanisms of enzyme-catalyzed reactions. The specific systems under investigation are the in vitro photosynthetic system composed of isolated chloroplasts, ferredoxin, and hydrogenase (CFH) and the enzyme-catalyzed conversion of cellulose to glucose. The CFH system is capable of the simultaneous photoproduction of hydrogen and oxygen when irradiated with visible light. Experimental progress includes the first measurements of the light saturation curves of biophotolysis of water and the first demonstration of the simultaneous photoproduction of hydrogen and oxygen by immobilized chloroplasts, ferredoxin, and hydrogenase. The key result is that the analytical shapes of the light saturation curves are not the same. A higher light intensity is required to saturate the hydrogen curve. These results challenge the Z-scheme concept of photosynthesis. A cellulase enzyme system is being investigated for the conversion of cellulose. An immobilized enzyme has been shown to maintain long-term stability and high activity for this application.

Chemistry Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $2,110,000

112. BASIC AQUEOUS CHEMISTRY TO HIGH TEMPERATURES AND PRESSURES — 5.3 — 02-01
R. H. Busey, R. E. Mesmer, H. F. Holmes, D. A. Palmer, W. L. Marshall

This program is directed toward the goal of a broad and detailed understanding of chemical processes occurring in aqueous systems to high temperatures and pressures. Such information relates to the safe and efficient operation of energy production, steam generation, fuel reprocessing, and waste disposal facilities as well as to the extraction of heat and materials from natural resources. Specialized techniques are employed in calorimetry, conductance, potentiometry, spectrophotometry, isopiestic and phase equilibrium studies at temperatures generally to 300°C and at modest pressures and sometimes to 800°C and 4000 bars. Species identification, thermodynamic properties and equilibrium stability information are obtained but some new emphasis will be placed on structural and detailed quantitative information from neutron and Raman scattering. The most significant scientific and practical contributions have been made with respect to the following: the ionization reactions of water and weak acids and bases; the association of 1:1 chlorides; the hydrolysis of metal ions; the phase behavior of oxides, sulfates and phosphates; excess thermodynamic quantities for chlorides and sulfates; and models for the pressure and temperature dependencies of chemical equilibria.

Chemistry Division, ORNL, continued

113. HETEROGENEOUS CATALYSIS RELATED TO ENERGY SYSTEMS — 2.2 — 02-01

S. H. Overbury, M. L. Poutsma

The technique of low energy ion scattering as a surface specific structural tool is being developed and applied to the study of clean and adsorbate covered single crystal surfaces of catalytic interest. Comparison of the experimentally observed energy and angle dependencies of the scattered ions with computer simulations allows for quantitative descriptions of surface structure. The information content from alkali metal ions (Li^+,K^+) exceeds that from inert gas ions because of their lower neutralization probability. These methods are being applied especially to adatoms such as O and C on clean Mo(100). These adatoms have been shown to occupy the four-fold sites at a perpendicular height of 0.3 Å above the surface.

114. ORGANIC CHEMISTRY AND THE CHEMISTRY OF FOSSIL FUELS — 7.1 — 02-01

M. L. Poutsma, E. W. Hagaman,
B. M. Benjamin, R. R. Chambers,
L. L. Brown

This experimental program is designed to determine the structure and reactivity of coal. The key spectroscopic technique being used for native and chemically modified coals is solid-state CP/MAS ^{13}C NMR with particular emphasis on developing the technique for use in a quantitative reliable manner. Diagnostic reactions for structural features being used include C-C bond cleavage induced by electron donors, C-H deprotonation induced by carbanions, and excision of aliphatic connecting groups by acid-catalyzed transalkylation. Mechanistic description of the thermal decomposition pathways of key structural units in coal has been advanced by use of appropriate model compounds; the role of diffusional restraints is being probed by use of surface-attached model compounds.

115. MOLTEN SALT CATALYSTS FOR CLEAN FUEL SYNTHESIS — 4.6 — 02-01

C. P. Smith, A. S. Dworkin, A. C. Buchanan, III, S. P. Zingg

This research elucidates the respective roles of redox and acid/base functionality in the catalytic reactions of arene hydrocarbons. Liquid metal halides at 25-150°C serve as catalysts. For the purpose of basic investigations these liquid catalysts have the advantage over solid catalysts that key catalytic properties, such as redox potential and Lewis acidity, can be varied over wide ranges in an accurate and reproducible way. Current experimental work includes an investigation of the formation reactions of selected arene radical cations (reactive intermediates in redox catalysis) and the kinetics of their decay reactions in $SbCl_3$-rich melts as functions of concentration, temperature, and the redox potential of the melt. These reactions are studied by fast optical spectroscopy and electrokinetic methods. In another investigation the activity and selectivity of Ga(III)/Ga(I) halide mixtures with respect to arene H-transfer reactions are being studied by *in situ* NMR spectroscopy and byproduct analysis following quench and separation.

Chemical Energy

Chemical Technology Department
Pacific Northwest Laboratory
P. O. Box 999
Richland, Washington 99352

Total $450,000

116. HYDROGENATION MECHANISMS OF COAL — 2.1 — 02-01

James A. Franz and Russell D. Barrows

This program is a basic research program directed at determining the energetics and mechanisms of free radical reactions related to thermal dissolution of coal in hydrogen donor media. Relative rates of radical rearrangements, atom transfer reactions, fragmentation reactions and change transfer reactions are being determined, with absolute rates determined by kinetic laserflash spectroscopy for key atom transfer reactions. The cyclization of ortho-allylbensyl radical to 2-indanylmethyl radical, for example, is used as an intramolecular free radical "clock" to compare atom transfer rates to benzylic radicals, thereby determining the relative donor strength of a wide variety of coal-related donors. Thermochemical values of select radicals are being determined using ESR of equilibrating radical mixtures, allowing estimates of difficultey observed radical rearrangements.

117. THERMOCHEMICAL CONVERSION OF SOLID WASTES INTO LIQUID FUELS — 1.8 — 02-01

D. A. Nelson, J. A. Russell, S. D. Landsman, P. M. Molton

The purpose of this research is to determine the reaction mechanisms involved in biomass liquefaction in aqueous media at elevated temperatures. Due to the complexity and variability of composition of biomass, the liquefaction of pure cellulose is now being studied. More than 90 components of the cellulose liquefaction product can be identified by gas chromatography-mass spectroscopy. Particular emphasis is now directed toward the aromatic products of the liquefaction product. The identification of alkyl substituted benzoquinones and benzenediols is quite interesting since their formation involves aldol condensation followed by a reduction-oxidation mechanism. Reactions occurring after formation of the cellulose liquefaction product apparently include oligomerization by auto-oxidation. The cellulose product oil shows rapid viscosity increases not associated with water or solvent loss; differential scanning calorimetry is consistent with nonlinear, branched oligomer formation.

Chemical Energy

Chemical and Instrumental Analysis Division
Pittsburgh Energy Technology Center
P. O. Box 10940
Pittsburgh, Pennsylvania 15236

Total $80,000

118. VIBRATIONAL SPECTROSCOPIC STUDIES OF COAL CONVERSION CATALYSTS
John M. Stencel

1.0 02-01

Research during the current year has concentrated on understanding molybdenum-support and tungsten-support interactions in Mo/Al_2O_3, W/Al_2O_3, $Ni-Mo/Al_2O_3$, and $Ni-W/Al_2O_3$ catalysts. Raman spectroscopy is the primary tool used to define molecular speciation for catalysts in which Mo, W, and Ni concentrations have been varied systematically. Additional information concerning the influence of concentration of metals on the vibrational frequencies of molecular species is obtained by chemical modification of the catalyst surface structure and by low temperature experiments. Raman experimentation is supplemented by data from other bulk and surface sensitive techniques, such as X-ray diffraction, X-ray photoelectron spectroscopy, and ion scattering spectroscopy. Correlations are made with catalytic reaction data to provide insight into structural and chemical factors that influence catalytic activity.

Radiation and Surface Physics Research Department
Sandia National Laboratories/Albuquerque
P. O. box 5800
Albuquerque, New Mexico 87115

Total $160,000

119. REACTION KINETICS OVER SINGLE CRYSTAL CATALYSTS
D. Wayne Goodman

1.6 02-01

The goal of this research is to develop an understanding of surface catalyzed reactions at the molecular level using the full complement of modern surface probes. Of primary importance are those reactions relating to the synthesis of hydrocarbons from H_2 and CO. The experimental work includes the determination of reaction kinetics of hydrocarbon formation and rearrangement over single crystal catalysts. The work is carried out in a specially built ultra-high vacuum apparatus allowing both kinetic measurements and surface analysis. Recent studies have addressed the role of potassium promoters in nickel catalysts for methanation. High-pressure kinetic measurements of this reaction over a Ni(100) catalyst containing submonolayer quantities of potassium adatoms have been combined with detailed surface analysis before and after reaction. Potassium decreases the rate of methane formation and increases the rate of higher hydrocarbons relative to the clean Ni(100) catalyst. Similar results have been reported for supported nickel catalysts suggesting that support effects play a small role in catalytic promotion by potassium.

Research Division
Solar Energy Research Institute
1617 Cole Boulevard
Golden, Colorado 80401

Total $150,000

120. BASIC RESEARCH IN SYNTHESIS AND CATALYSIS
J. C. Smart, D. L. DuBois and
C. J. Curtis

1.5 02-01

This basic research program involves the synthesis, characterization and reaction studies of transition metal coordination complexes and organometallic compounds for the photoconversion of N_2, CO, CO_2, H_2O and related substrates to fuels and chemicals. It includes structural, spectroscopic and mechanistic studies with the goal of understanding the interrelationship of molecular geometry, electronic structure and catalytic reactivity in photochemical and photoelectrochemical transformations. Designed organometallic synthesis has yielded new bi- and trimetallic complexes with bridging fulvalene, s- and as-indacene, and trindene ligands of Ti, Zr, Ta, Mo, and Mn. Spectroscopic and photochemical studies of Co and Ni metallofulvalene complexes is contributing to an understanding of their electronic structures and the potential utility of their low-lying excited states in photocatalysis. Photoelectrochemical N_2-fixation studies involve the synthesis and characterization of surface bound polymer-pendant phosphine molybdenum(0) dinitrogen complexes using combined FT-IR and electrochemical techniques.

Separations and Analysis

Ames Laboratory
Iowa State University
Ames, Iowa 50011

Total $990,000

121. HYDROMETALLURGICAL PROCESSING — 1.6 — 02-02
Renato G. Bautista

The development and understanding of hydrometallurgical methods of recovering metals to include dissolution (leaching), separation and concentration (ion exchange, solvent extraction, and membrane separation) and metal reduction from solutions (cementation, precipitation, and electrolysis) based on the equilibria, mechanisms, kinetics, and transport properties of the chemical reaction system are the related activities which are the principal objectives of this research program. The research projects presently being completed include: the kinetics of the dissolution of pyrrhotite and pentlandite by ferric sulfate and sulfuric acid and the prediction of the concentration changes of the various species in solution during the dissolution process using the partial equilibrium model; the separation and concentration of ppm platinum chloride solution using a supported liquid membrane impregnated with trioctylamine as a mobile carrier and the elucidation of its mass transfer mechanism for permeation through the membrane; and the modeling of the electrowinning of dilute copper sulfate solution using a fluidized bed electrochemical reactor.

122. ANALYTICAL MASS SPECTROMETRY — 0.9 — 02-02
R. J. Conzemius, H. J. Svec

The objective of this project is to develop viable analytical techniques for a wide range of analytical requirements based on mass spectrometry of solids. The general approach involves the direct excitation of specimens to the ionic state using high energy processes such as a high frequency spark, a focused laser beam, and other plasma ion sources. The advantage of this approach is that it provides analytical characterization including speciation of surface contaminants as well as elemental analysis without requiring specimen dissolution or chemical treatment and with minimum sample preparation. The ultimate goal of the work is to realize an analytical system which is an absolute detector for all elements in the periodic table providing quantitative accuracies without the need for standards for major elements as well as those at ultratrace levels. Studies are also guided by the necessity to avoid excessive instrumentation costs.

123. ANALYTICAL SPECTROSCOPY — 4.7 — 02-02
V. A. Fassel, A. P. D'Silva,
R. N. Kniseley, J. F. McClelland
E. DeKalb

This effort is devoted to the systematic observation of spectroscopic phenomena with the ultimate goal of utilizing these observations for devising new spectroscopic analytical concepts that offer promise of solving singularly difficult analytical problems that either exist now or are likely to arise in the future in the various fields of energy generation, the conversion of coal to liquid and gaseous fuels, solid state materials research and in environmental pollution. Emphasis is being placed on: (a) novel applications of electrical plasmas as vaporization-atomization-excitation-ionization sources for analytical atomic emission and fluorescence spectroscopy; (b) analytical applications of highly selective energy transfer processes from x-ray and laser beams to trace constituents in solid materials, leading to optical emission, e.g., x-ray or laser excited optical luminescence; (c) selective energy transfer from gaseous metastable species to trace level gaseous organic or inorganic constituents, with the intent to devise new analytical concepts; and (d) photoacoustic spectroscopy analytical techniques.

Ames Laboratory, continued

124. ANALYTICAL SEPARATIONS AND CHEMICAL ANALYSIS — 1.9 — 02-02
J. S. Fritz

A major effort is underway to improve our new method of Ion Chromatography so that complex mixtures of inorganic anions and cations can be separated and analyzed with the same facility that is possible in organic chromatography. Research on ion-exchange resins is designed to provide better resins for chromatography and to give a better understanding of the important scientific problem of resin selectivity. New methods are being developed for the selective concentration of various organic compounds prior to chromatographic analysis. Work is progressing on an improved statistical theory of chromatography which should correct some inadequacies of prevailing theories and provide a better foundation for chromatography.

125. MASS SPECTROMETRY OF PLASMAS — 1.5 — 02-02
R. S. Houk

The general objective of this research is to develop, evaluate, and characterize ionization techniques with potential value for analytical mass spectrometry (MS). Current efforts concentrate on improving techniques for extracting and mass analyzing ions from inductively coupled plasmas (ICPs). The value of this ion source for elemental and isotopic analysis of solutions on a rapid, direct basis is being demonstrated. Various alternate techniques for introducing samples are being studied with the ICP-MS device as an element-selective, isotopically-sensitive detector. These sample introduction methods include electrothermal furnaces or arc discharges for direct vaporization of solids and liquid chromatographic separations for determining elemental speciation via isotopic tracing experiments. Mass spectra of amino acids and other polar, nonvolatile organic compounds can be obtained directly from aqueous solutions provided ICP conditions are properly "cooled". Temperatures, ion and electron densities, and energy transfer processes in ICP are also being modeled and studied experimentally by mass spectrometric measurements.

126. LASERS IN ANALYTICAL CHEMISTRY — 4.6 — 02-02
E. S. Yeung

This program is aimed towards the development of new analytical techniques relevant to pollution monitoring, combustion diagnosis, and material evaluation in energy production. New spectroscopic concepts and instrumentation, particularly those involving lasers, are studied so that analytical methods can gain in sensitivity, selectivity, accuracy, and speed. Specific areas of concern include (1) the development of the laser microprobe for atomic spectroscopy on surfaces; (2) new optical detectors for liquid chromatography suitable for complex samples; (3) Raman methods and two-photon methods applied to analytical problems; (4) photoacoustic and interferometric concepts for improved absorption measurements; and (5) laser-induced chemiluminescence for specific gas analysis. Investigations include the fundamental principles behind the measurements, the evaluation of the analytical potentials, and the demonstration of the analytical method in representative samples.

61

Separations and Analysis

Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Total $1,300,000

127. SEPARATION SCIENCE RELATED TO NUCLEAR AND HYDROMETALLURGICAL TECHNOLOGY — 7.7 — 02-02

E. P. Horwitz, P. R. Danesi, H. Diamond, D. Kalina, L. Kaplan, P. G. Rickart, C.W. Mason

This program has as its objectives the development of new organic extractants for the separation of metal ions and the study of the underlying principles involved in the transfer of metal ions from an aqueous to an organic environment. Knowledge gained from these basic studies is applied to the development of new and improved separation methods of importance in nuclear fuel reprocessing, nuclear waste processing, and the recovery of strategic metals from low grade domestic sources. Major areas of investigation are: (1) The synthesis and characterization of new extractants for metal ions. This involves equilibrium studies, rate and mechanism studies of interfacial mass transfer, and elucidation of solution structures of metal extractant complexes. (2) The basic physical chemistry of supported liquid membranes. Systems are studied with respect to the hydrodynamic, diffusional, and equilibrium parameters which influence the permeability rates of metal ions. Major subdivisions are modeling of flat sheet and hollow fiber systems, multielement separations, and development of energy-efficient recovery systems for metal ions.

128. STUDY OF ATMOSPHERIC TRACE GASES BY MASS SPECTROMETRY — 1.3 — 02-02

C. Stevens

The carbon isotopic composition of atmospheric methane and its natural and anthropogenic sources is being measured to establish the relative distribution of these sources. In addition we are collaborating with Dr. R. Rasmussen of the Oregon Graduate Center in analyzing the isotopic composition of methane in old air samples collected in both hemispheres since 1978. Changes in the composition reflect changes in the fluxes of enriched or depleted ^{13}C-methane. The purpose of these measurements is to provide clues for causes of an increasing concentration of atmospheric methane; whether it is produced by increasing source fluxes or a decreasing rate of removal from the atmosphere. The results of this study bear on the extent of the methane contribution to the so-called "greenhouse effect" and its effect on future climate changes.

129. SEPARATIONS OF COAL MACERALS AND OTHER FOSSIL FUELS — 2.0 — 02-02

R. E. Winans, G. R. Dyrkacz, C. A. A. Bloomquist

The major objectives of this program are to separate and characterize coal macerals and to develop new separation techniques to achieve this end. A major problem in coal science is the complexity of the substance. However, we have made an important step in reducing this problem by separating coals into their maceral constituents by density gradient centrifugation. Significant differences in chemical structure and reactivity have been discovered among the various maceral groups and also within maceral groups. These findings are important in that they provide insight into the behavior of macerals in coal processes. Surface properties of coal macerals are being studied in a search for new and more efficient methods of separation and identification.

Separations and Analysis

Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973

Total $215,000

130. APPLICATIONS OF NUCLEAR METHODS TO ANALYSIS — 2.5 — 02-02
C. Harbottle, E. V. Sayre, R. W. Stoenner

This program is concerned with the extension and improvement of nuclear methods of elemental analysis, particularly methods that permit the determination of many components (including trace impurities) quickly and efficiently, and with the development of computer-based multivariate statistical analysis which will permit the efficient and effective analysis of large assemblages of such analytical data. These methods are being applied to a wide variety of materials for which geographic origins are of significant interest. The effects of geochemical processes on trace element patterns are being investigated in several natural materials and artifacts made from them. Studies of the accuracy and precision of standardization in activation analysis are an important part of the program. The improved proportional counter method for carbon-14 measurement in samples as small as 10 mg is being applied to marine sediments in an attempt to account for the carbon dioxide inventory of the world.

Separations and Analysis

Department of Applied Sciences
Brookhaven National Laboratory
Upton, New York 11973

Total $280,000

131. SPECIFIC MOLECULAR PROPERTY DETECTORS FOR CHROMATOGRAPHIC ANALYSIS — 1.7 — 02-02
J. Gaffney, E. Premuzic

This research effort is developing novel specific molecular property detectors for use in gas and liquid chromatography. Detection schemes are being devised which simplify the separation analyses by increasing the detector response for the specific molecules of interest while reducing the background noise from potential interferences. Areas of application range from process monitoring to trace analysis in environmental and biomedical investigations. The program is currently developing monitors for specific hydrocarbons and hydrocarbon classes. Far-ultra violet (130-300nm) circular dichroism is under investigation as a means of monitoring optically active hydrocarbons eluting from a gas chromatograph. This device will use the National Synchrotron Light Source (NSLS). The spectral and thermal properties of ozone-chemiluminescence as a means of monitoring hydrocarbon classes (e.g., reduced sulfur compounds, olefins, etc.) as well as photothermal laser spectroscopies are also being investigated as selective and sensitive devices for chromatographic detection.

Department of Applied Sciences, BNL, continued

132. CYCLIC SEPARATIONS PROCESS RESEARCH — 1.6 — 02-02
F. B. Hill

The purposes of this program are to obtain an understanding of the characteristics and basis of operation of cyclic separation processes as a class, and to explore the feasibility of using these processes to perform specific separations important in the energy field. The cyclic processes of interest include pressure and temperature swing adsorption, parametric pumping, cycling zone adsorption and various forms of preparative chromatography. Applications presently under study involve hydrogen isotope separations of concern in fusion reactor fuel processing and in heavy water reactor technology, and helium extraction from natural gas. Future work will include applications such as hydrogen recovery and purification, and ion exchange separations useful in radwaste applications. Elements of the program include development of the theory of cyclic processes, measurements of equilibrium and kinetic properties of selected fluid-solid separation systems, measurement of the characteristics of cyclic separation processes employing these systems, and process design and evaluations studies.

Physics Department
Brookhaven National Laboratory
Upton, New York 11973 — Total $310,000

133. ANALYTICAL TECHNIQUES WITH SYNCHROTRON RADIATION AND ION BEAMS — 4.0 — 02-02
K. W. Jones, H. W. Kraner, B. M. Gordon

This program develops new analytical techniques for elemental analysis using synchrotron radiation from the National Synchrotron Light Source. Equipment is being designed and fabricated to produce a focussed x-ray beam with a spatial resolution around 10 μm. Techniques for precise trace element measurements with minimum detectable limits down to 10^{-9} g/g are being developed concurrently for both bulk and microanalysis. A searching test of the new methods is made by comparison of the results obtained with synchrotron radiation with those obtained by other methods. These tests require the application of the techniques to samples obtained from a variety of energy-related fields. The use of synchrotron radiation for elemental identification is supported by the use of nuclear ion-beam analysis which makes available complementary analytical techniques that are used to corroborate and extend the synchrotron radiation results.

Separations and Analysis

EG&G Idaho, Inc.
Idaho National Engineering Laboratory
P.O. Box 1625
Idaho Falls, Idaho 83415 — Total $65,000

134. SELECTED ELEMENTAL SEPARATION STUDY — 1.0 — 02-02
J.D. Baker and J.S. Jessup

The focus of this research is studying selective elemental extractants which show promise in partitioning valuable metals from aqueous solutions. This year, the extraction behavior of Mo from HNO_3 was studied using dihexyl-N, N-diethylcarbamoylmethylphosphonate. Distribution coefficients were measured as a function of contact time, concentration of Mo, HNO_3, NO_3^- and extractant, and extraction temperature. There appears to be a Mo species change above ~6M HNO_3 which was an extractable moiety. Thus far, our research has been limited to organophosphorus extractants. Recently we extended these studies to include analogous organosulfur compounds.

84

Separations and Analysis

Exxon Nuclear Idaho Co., Inc.
Idaho National Engineering Laboratory
P.O. Box 2800
Idaho Falls, Idaho 83401

Total $100,000

135. NEGATIVE ION MASS SPECTROMETRY — 1.0 — 02-02
J.E. Delmore

This program is studying two ionization processes for application to negative ion mass spectrometry: negative surface ionization and electron capture. Surface ionization studies are focused on systems where the species of interest is chemisorped on a low work function surface, followed by thermal desorption. To date, ions studied by this method include Cl^-, Br^-, I^-, BO_2^-, CN^-, CHO^- and H^-. Ionization efficiency has been increased by several orders of magnitude using this technique. A unique electron capture ion source using crossed electric/magnetic fields has been theoretically modeled, designed, constructed and tested. This ion source forces electrons into a cycloidal orbit to reduce the kinetic energy to thermal values. The thermalized electrons are readily captured by gas molecules to form negative ions without the high pressure system otherwise required for electron capture mass spectrometry. Refinement of both the experimental model and instrumentation is the major thrust of the program for the next year.

Separations and Analysis

P Division
Los Alamos National Laboratory
University of California
P. O. Box 1663
Los Alamos, New Mexico 87545

Total $170,000

136. THE FORMATION AND PROPERTIES OF COMPLEXES OF HELIUM AND HYDROGEN ISOTOPES — 1.5 — 02-02
R. D. Taylor

The conditions for formation and the properties of a metastable, bound-state complex of ^3He and tritium are under study. T_2 decays with a half life of 12.3 years ultimately producing a pair of ^3He atoms. However, vapor pressure-time measurements show that the ^3He formed in liquid T_2 is retained in the liquid in an amount far exceeding the ordinary solubility. This complex, once formed, is found to be unstable in the gas phase, but it is virtually stable in liquid or in solid tritium. Preliminary data for solid T_2 at 20.0 K suggest that the newly formed ^3He is also bound. The electrical conductivity of solid T_2 containing the complex shows an initial decline of about a factor of three from the conductivity of the liquid. After a few days, this conductivity is about 100 times less. A new cell is under development that will allow pressure buildup measurements of liquid or solid T_2 without the complication of gas phase corrections. Other time-temperature measurements to characterize the complex include magnetic susceptibility and compositional studies of successive portions of gas removed from the cold cell.

Separations and Analysis

Mound Facility
P.O. Box 32
Miamisburg, Ohio 45342

Total $745,000

137. ISOTOPE SEPARATION RESEARCH AND DEVELOPMENT — 3.75 — 02-02
W. M. Rutherford, B. E. Jepson, E. D. Michaels, W. R. Wilkes

This program is concerned with the investigation of chemical exchange and liquid phase thermal diffusion as techniques for stable isotope separation. The chemical exchange work is directed toward finding significant equilibrium isotope effects in metal isotope exchange reactions with an emphasis on macrocyclic complexants, and towards the development of two-phase isotope exchange processes for practical separations. The liquid thermal diffusion work is directed, in part, toward developing a basic understanding of the behavior of liquid phase thermal diffusion columns and, in part, toward gaining experimental information about the isotopic thermal diffusion factor in the liquid phase.

138. MOLECULAR SCIENCE RESEARCH — 4.8 — 02-02
W. L. Taylor, G. T. McConville, R. W. York

The objective of this research is to investigate the physical properties of isotopes and their mixtures. To obtain a more complete understanding of gaseous mixtures of hydrogen isotopes, in particular, the mechanisms for isotopic exchange in such mixtures, measurements of the formation of DT in mixtures of D_2+T_2 are being made as a function of pressure, initial T_2 concentration, and temperature. The interaction with D_2 is very complex and the presence of excited state molecules plays a definite part in the reaction. Such information will be useful in design criteria for fuel handling systems in the controlled-thermonuclear power program. Total and differential cross sections are being measured for the permanent gases with supersonic molecular beams. The data are analyzed to yield the fundamental interactions of the colliding species. The temperature range of diffusion measurements in binary gas mixtures is being extended to ~2500°C by means of a Ta/W diffusion cell operating in a vacuum furnace. The thermodynamics of the thermal diffusion process is under study in a "swing separator" instrumented with thermistors for "in situ" and real time analysis of the separation process. Ortho- and para-deuterium are being separated in a cryogenic adsorption column and will be made available to the Stable Isotope Inventory Program.

Separations and Analysis

Analytical Chemistry Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $1,300,000

139. R&D IN SECONDARY ION MASS SPECTROMETRY — 2.1 — 02-02
W. H. Christie, R. E. Eby, P. J. Todd

Sputtering has become one of the most intensely investigated methods for producing ions for mass spectrometric analysis. This technique, secondary ion mass spectrometry (SIMS), provides a unique capability in areas of surface analysis, diffusion studies, depth profiling, nonvolatile organic materials analysis, as well as providing isotopic and elemental information. The overall objectives of this program are: 1) developing state-of-the-art methods for acquiring, processing, and quantifying SIMS data; 2) applying this new technique to the solution of surface analytical problems in on-going DOE research programs; and 3) the development of instrumentation and methodology to investigate the suitability of SIMS in new analytical areas such as the characterization of non-volatile organic materials. A secondary ion source developed for work with organic species will be used in conjunction with an MS/MS mass spectrometer to investigate the chemistry and physics of secondary ion emission from involatile organic species.

140. MASS SPECTROMETRY R & D FOR ORGANIC ANALYSES — 2.4 — 02-02
G. L. Glish, P. J. Todd,
E. H. McBay

This research is aimed at improving and extending the application of organic mass spectrometry to analytical problems. Included are development of instrumental techniques to advance the study of the chemistry and physics of gas phase ions; the study of the processes involved in desorption ionization; and study of the chemistry and physics of gas phase ions to arrive at a better understanding of the fundamental processes involved. Heavy emphasis is currently placed on the technique of mass spectrometry/mass spectrometry (MS/MS), both as an analytical tool and in developing instrumentation for new applications. Ionization of involatile organic compounds is being investigated, often in conjunction with MS/MS. By selecting an ion of interest and injecting it into a collision cell filled with a suitable gas, fragmentation characteristic of the compound in question is induced. This, the MS/MS technique, offers a powerful tool both for study of gas phase interactions and for unambiguous identification of compounds from isomeric or other mixtures.

141. ADVANCED SPECTROSCOPIC METHODS FOR CHEMICAL ANALYSIS — 2.5 — 02-02
L. Hulett, J. Dale, T. Rosseel

The objective of this research is to explore new physical effects and to utilize facilities unique to ORNL as spectroscopic tools; also, methods involving more conventional principles are upgraded as improvements in the older technologies become available. Monoenergetic positron spectroscopy is being evaluated for its ability to determine surface and bulk properties of materials. X-ray fluorescence spectra, generated in heavy ion bombardment experiments, have been found to be sensitive to chemical properties of metals and alloys. Development of improved techniques for such problems as determining specimen thicknesses, sizes, and composition, using the transmission electron microscope, will be initiated. X-ray photoelectron spectroscopy will be combined with scanning electron microscopy. Fast turnaround methods for asbestos assay, using x-ray diffraction, will be investigated. Collaboration involves the ORNL Physics, Chemical Technology, and Metals and Ceramics Division.

Analytical Chemistry Division, ORNL, continued

142. RESEARCH DEVELOPMENT & DEMONSTRATION OF ADVANCED CHEMICAL MEASUREMENT TECHNIQUES — 3.6 — 02-02
H. Ross, M. Ramsey, R. Shaw, W. Whitten, J. Young

Advanced technology from a variety of disciplines is being brought together to develop unique analytical measurement systems. These systems have a generic application to analytical problems in research, industry, and energy technology. The major area of study is spectroscopy. Fourier transform microwave spectroscopy is a new, high resolution technique that has broad application potential. A technique that will allow the rapid qualitation and quantitation of complex mixtures, optoacoustic spectroscopy, is being applied to matrix isolated materials. A novel piezoelectric detector is under development for this work. The application of fiber-optic waveguides to analytical chemistry is also being studied. This work is concerned with spectral resolution in both the time and space domains. Ongoing studies of laser excited optogalvanic spectroscopy indicate several practical advantages with this method. Time-resolved laser-excited fluorescence, delayed lasing, and laser ablation for solid sampling are also under investigation. A project to examine the analytical utility of molecular beams in spectroscopy has been initiated.

143. MASS SPECTROMETRIC RESEARCH AND DEVELOPMENT FOR INORGANIC ANALYSES — 2.6 — 02-02
R. L. Walker, H. S. McKown, D. H. Smith, D. L. Donohue

The aim of this research is to improve the analytical precision and accuracy of isotope ratio measurements by mass spectrometry. Studies have been performed to improve the precision of conventional thermal ionization measurements by using an internal standard, or "double spike" method for uranium and plutonium analyses. Successful implementation has increased the measurement precision by a factor of 3-5, to below 0.1% RSD for uranium isotopes. The shortage of high purity spike material such as ^{236}U and ^{244}Pu is the only limitation on widespread use of this technique. Laser-induced resonance ionization techniques have been studied as a way to improve the accuracy of isotopic analyses for elements with overlapping isotopes. Useful information has been obtained with the rare-earth elements Nd, Sm, and Eu, and preliminary results for the system U:Pu:Am are very encouraging. An ion optical bench facility has been constructed and used to characterize and optimize ion detectors for pulse counting applications.

Separations and Analysis

Chemical Technology Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $2,000,000

144. CHEMICAL SEPARATIONS FOR LOW GRADE SOURCES — 3.9 — 02-02

R. M. Canon, S. D. Clinton, D. J. Pruett

Fundamental investigations are carried out on chemical separations important to the recovery of metal values from low grade domestic sources, including waste streams. These include the study of mechanisms of ion exchange, crystallization and solvent extraction systems, as well as extraction of metals from the source materials. Recent investigations have concentrated on separations and extractions utilizing chloride chemistry in both aqueous and nonaqueous (aprotic) systems. Studies in aqueous systems include multicomponent metal solubility determinations at various hydrogen chloride activities and the use of HCl gas sparging for crystallization from multicomponent systems. The high chloride activities possible in aprotic solvents make these systems attractive as extractants and as separation tools. Tests have concentrated on the determination of phase diagrams for selected ternary systems of solvent-metal chloride-water.

145. CHEMICAL SEPARATIONS BY COMPLEXATION PHENOMENA — 5.0 — 02-02

C. F. Coleman, W. J. McDowell

Basic scientific understanding of methods for separating mixed elements, compounds, or aggregate materials is being obtained by systematic and fundamental studies of equilibria and mechanisms and of the properties of the components in selected separations systems. The present emphasis is on solvent extraction and ion exchange systems, which are well defined and of wide-spread concern. A major aim is understanding of the relationship between reagent structure and selectivity for particular ions or molecules, so that agents can be designed for improved selectivity, kinetics, and phase behavior. Multidentate extractants, including chelating and macrocyclic compounds, are emphasized because their known complex-forming behavior gives basis for designing specificity into reagents. Detailed studies include: the effects on a range of functional groups when they are attached to carrier molecules or resin skeletons; synergistic combinations of different functions; and elucidation of the structures of adducts of metals with ligands that are known to be selective.

146. CHEMICAL SEPARATIONS FOR TRITIUM — 1.8 — 02-02

P. W. Fisher, S. D. Clinton

This program seeks to understand the fundamental physical and chemical aspects of tritium separation ultimately useful for fusion and fission energy systems. The major current efforts include the separation of tritium from molten lithium, separation of tritium from solid materials, and measurement of equilibrium and transport properties for tritium in solid materials. In earlier phases of this program it was found that sorption of tritium from molten lithium could be achieved through use of yttrium sorbers. These materials are able to reduce the tritium level to below 1 ppm. Fundamental physical properties, like diffusivities and solubilities, are obtained for yttrium-containing materials through a combination of experimentation and mathematical modeling. New classes of yttrium-bearing materials are being analyzed and tested to evaluate these findings.

Chemical Technology Division, ORNL, continued

147. CHEMISTRY OF ACTINIDES AND FISSION PRODUCTS — 3.1 — 02-02
L. M. Toth, D. J. Pruett

The chemistry of actinides and of fission products are investigated with emphasis on the properties that affect separation and partitioning in the nuclear fuel cycle. The broad scope of subjects includes photochemical studies, the structures and properties of polymer materials, solvent extraction and co-extractions, and the induction times and precipitation in pseudo stable process and waste streams. Recent studies have concentrated on the solvent extraction of heptavalent technetium and rhenium in nitric acid systems with and without uranium, and on the photochemical reduction of heptavalent technetium to the V and IV states in nitric and hydrochloric acids. New research will include the photochemistry of low temperature uranium and plutonium frozen solutions or salts, and the catalytic effects of Pu(IV) on actinide redox reactions.

148. CHEMICAL AND PHYSICAL PRINCIPLES IN MULTIPHASE SEPARATIONS — 5.3 — 02-02
R. M. Wham, C. H. Byers,
J. S. Watson

Fundamental chemical engineering investigations include new concepts and basic understanding of multiphase separation methods. Fluidized and expanded beds are stabilized by the imposition of an electric field, thus exhibiting the desirable sorption characteristics of fixed beds, while the pressure drop is approximately half the fixed bed. The applicability of this principle to a novel method for moving bed sorption is under study. Mass transfer enhancement in dispersed-phase systems by forcing the oscillation of small droplets in a continuous medium is being investigated. Preliminary results show that droplet motion can be forced by an oscillating electric field. A study to investigate separation phenomena associated with the distribution of a solute between a liquid and solidified (frozen) solvent has been initiated. Preliminary results indicate that a chromatographic separation of selected solutes is possible.

Separations and Analysis

Chemistry Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $330,000

149. FUNDAMENTALS OF SEPARATIONS CHEMISTRY — 2.1 — 02-02
J. H. Burns, C. F. Baes, Jr.

The purpose of this research is to obtain basic information about solvent-extraction systems that may lead to improved processes for recovery of strategic materials for national energy needs. The approach is to investigate known successful processes with the aim of understanding on a molecular level the mechanism by which they operate and to determine which variables of reactivity and structure are important to their success. Typical systems for the extraction of uranium by organophosphorus liganda are being analyzed by X-ray diffraction of solids and liquids, and the structural information obtained is being used to develop structural criteria for solvent extraction which will have a general applicability. These criteria are being used in the design of more effective extraction reagents for uranium and could provide a guide for the development of new techniques for the separation of other metals.

150. MOLTEN SALT PROCESSES FOR HIGH LEVEL RADIOACTIVE WASTE — 1.1 — 02-02
F. J. Smith

The basic chemistry that relates to high-temperature non-aqueous methods for extracting useful products from spent nuclear fuel is being developed. A major accomplishment of this program is the demonstration of the chemical feasibility of isolating significant quantities of non-radioactive palladium and rhodium as by-products from conventional processing of LWR or LMFBR fuel. Separation processes which utilize liquid metal and molten salt systems are chosen because of their inherent radiation and proliferation resistance. Partitioning of palladium, rhodium, and ruthenium between liquid magnesium and molten uranium-iron eutectic at 750°C provides excellent separations (separation factors greater than 10^6) and forms the basis for the recovery process. Currently being determined is the distribution behavior of palladium, rhodium and ruthenium bromides between the two immiscible liquid phases in the $AlBr_3$-KBr system. Other studies involve molten alkali-metal cyanide/liquid metal (Zn, Bi, Sn) systems.

Biology and Chemistry Department
Pacific Northwest Laboratory
P. O. Box 999
Richland, Washington 99352

Total $70,000

151. FUNDAMENTAL PHASE PARTITIONING IN SUPERCRITICAL FLUID CHROMATOGRAPHY
R. D. Smith, B. W. Wright, H. R. Udseth

0.6 02-02

The goal of this program is a fundamental understanding of the kinetic and thermodynamic constraints upon partitioning of a solute between a supercritical fluid and a supported phase. The program involves investigation of fluid phase solubilities and phase partitioning kinetics relevant to supercritical fluid chromatography and extraction phenomena. Phase partitioning is being studied using direct fluid injection-mass spectrometry and various optical techniques. The program is directed at gaining an understanding of polar supercritical fluids and solute systems and the kinetic and thermodynamic limitations upon separations in supercritical media. These systems include supercritical ammonia, sulfur dioxide, and mixed fluid systems with solutes covering a wide range of polarity. Results of these studies will be compared with both theoretical methods for prediction of fluid phase solubilities and actual chromatographic separations for model systems.

Separations and Analysis

Chemical Technology Department
Pacific Northwest Laboratory
P. O. Box 999
Richland, Washington 99352

Total $80,000

152. PYROCHEMICAL SEPARATIONS
L. L. Burger, L. G. Morgan

1.1 02-02

This research develops pyrochemical methods for chemical separations in the nuclear fuel cycle. Separation of constituents into chemical families where the forms and behavior are unique benefits nuclear fuel reprocessing & treatment of nuclear wastes. Pyrochemical processes remove the complication of the water molecule which largely determines conventional chemical behavior. Studies using molten alkali metal nitrate systems & glass slag reductions have been emphasized. Molten alkali metal nitrates are both an oxidizing and a complexing media. Distribution of actinides and fission products between the molten nitrates and the solid phases present have been determined for uranium-plutonium oxide fuels. Thorium-uranium oxide fuels were also studied. Recovery of noble metals, including silver, from a variety of source metals, including simulated nuclear wastes and various inorganic substrates or matrices, has been demonstrated using a glass slag reduction technique. Distribution of the noble metals between the source material, the molten flux, and the molten metal phase has been studied and the overall efficiency of recovery determined.

Radiological Sciences Department
Pacific Northwest Laboratory
P. O. Box 999
Richland, Washington 99352

Total $700,000

153. LASER-BASED ANALYTICAL TECHNIQUES — 1.4 — 02-02
B. A. Bushaw, J. H. Kaye and
R. A. Warner

The objective of this program is to develop and evaluate ultrasensitive and highly selective laser-based analytical techniques. Current experimental work involves evaluating the potential of the photon burst technique for analytical applications. In this method, an atomic beam orthogonally intersects a CW dye laser beam which is tuned to the proper frequency to induce resonant absorption and fluorescence. As each individual atom passes through the laser beam a sudden burst of photons is emitted in a very short time interval. An innovative detection method based on the distribution of time intervals between detected photons allows the density of atoms of individual isotopes in the atomic beam to be determined, independent of minor fluctuations in the laser power and independent of whether or not the laser is exactly tuned to the resonance frequency. To date this method has been applied to measurements of sodium and rubidium isotopes. It is planned to extend the technique to measurement of isotopes of other alkali and alkaline earth metals and then to other selected elements. Methods for analysis of real world samples by photon-burst techniques are also being explored.

154. ANALYTICAL MASS SPECTROMETRY RESEARCH — 3.3 — 02-02
R. L. Gordon, D. M. Robertson,
J. M. Kelley and J. J. Stoffels

This task develops new knowledge and techniques to extend the application of mass spectrometry to problems in chemical and isotopic analyses. The task elucidates physicochemical mechanisms responsible for efficient ion production in isotopic analysis by surface ionization mass spectrometry, develops methods for the control of surface work function of ion sources, develops techniques for application of mass spectrometry to real-time analysis, and establishes new ionization techniques. Surface analytical tools are used to establish physical and chemical properties of surface ionization sources and to identify chemical pathways responsible for ion production. The direct-inlet technique for real-time mass spectrometry uses innovations in ion sources, mass separators, and ion detectors. Laser-assisted ionization is being developed for new mass spectrometry ion sources.

Radiological Sciences Department, PNL, continued

155. ULTRASENSITIVE RADIOACTIVITY SPECTROMETRIC ANALYTICAL TECHNIQUES — 0.5 — 02-02
J. H. Kaye

The objective of this program is to develop new and improved ultrasensitive and selective radioactivity spectrometric techniques for analysis of radionuclides. The current study involves an evaluation of time-of-event counting, a method wherein the time at which each counting event occurs is recorded as well as its pulse height. A computer simulation method has been developed which allows a large number of simulated counting experiments to be generated and analyzed in a few minutes' time. A comparison between the real and simulated data was made to verify that no difference was discernable. Advantages of the simulation approach are that a great deal of time is saved and the parameters of each simulation case can be exactly specified. A number of different data analysis methods are being evaluated. With the computer simulation approach, a comparison is being made between the detection limits obtainable with the time-of-event data analysis methods and with conventional, grouped-data counting techniques. Effects due to detector background and detector efficiency are being determined.

156. ANALYTICAL ATOMIC ABSORPTION SPECTROMETRY RESEARCH — 1.3 — 02-02
D. L. Styris and J. H. Kaye

This program elucidates experimentally the mechanisms that control sample vaporization in furnace atomic absorption (FAA) spectrometry. Vaporization models that are developed from these results provide understanding of chemical treatment and furnace effects and thus establish the basis needed to help broaden and improve application of contemporary FAA spectrometric analysis. The neutral atoms, ions and molecular species that appear in vapor phases during the temperature rise of the furnace are monitored simultaneously by atomic absorption and mass spectrometric techniques. Correlation of results from these experiments with furnace temperature and application of chemical thermodynamic and kinetic data help to identify and characterize the controlling chemical and physical processes. Vitreous carbon, tantalum, and graphite furnace materials are being used presently in order to model the vaporization of the Group IIA elements in presence of these furnace materials.

Laser Research and Development Department — Total $100,000
Sandia National Laboratories/Albuquerque
P. O. Box 5800
Albuquerque, New Mexico 87115

157. LASER BASED ANALYTICAL METHODS — 1.0 — 02-02
A. Owyoung, A.V. Smith, J.P. Hohlmer

This research is directed toward the development of new, highly sensitive, species-specific laser-based analytical techniques with capabilities beyond the reach of conventional methods of analysis. To this end our program emphasizes (1) the determination of the utility and limitations of newly developed laser-based techniques (such as multiphoton ionization spectrometry, MPIS) in analytical applications, (2) the integration of such techniques with more conventional methods of anlaysis (such as mass spectrometry) to provide analytical capabilities of increased dimension, and (3) the exploration of entirely new laser-based concepts having potential utility for analytical applications. In the area of laser source development for MPIS we are now able to generate coherent vacuum ultraviolet radiation over the range 105-200 nm. A second-generation laser-ionization mass spectrometer is also being developed. This 1.0 meter time-of-flight instrument will allow the use of laser ionization and a molecular free-expansion jet and will be used to evaluate techniques for improving the sensitivity and selectivity of MPIS.

39-707 01337

84

Chemical Engineering Sciences

Division of Applied Sciences
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $230,000

158. TURBULENT COMBUSTION — 2.5 — 02-04
F. Robben, R. K. Cheng and L. Talbot

The effect of fluid mechanical turbulence on combustion is being studied experimentally for premixed fuel/air conditions in two idealized flow configurations: 1) turbulent boundary layer over a strongly heated wall where lean combustion occurs, 2) an unconfined v-shaped turbulent flame. Density and velocity fluctuations and several of their cross correlation parameters are measured using techniques based on laser Rayleigh scattering and laser Doppler velocimetry. These measurements are useful to characterize the features of the flame structures and their effects on the turbulent flow field. The initiation and development of combustion in the heated boundary layer are found to be dominated by the large-scale turbulence structures. Measurements of Reynolds stress in the v-shaped flame have shown that a mean-gradient transport model for production of turbulent kinetic energy is not appropriate for these flames.

Materials and Molecular Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Total $140,000

159. HIGH-PRESSURE PHASE EQUILIBRIA IN HYDROCARBON-WATER (BRINE) SYSTEMS — 2.1 — 02-04
J. M. Prausnitz

Experimental and molecular-thermodynamic studies are directed toward better understanding of vapor-liquid and liquid-liquid equilibria for systems containing hydrocarbons with water (or brine). Such systems are of interest in the fossil-energy industry. Toward a quantitative description of equilibria in aquifers, an experimental apparatus is used to measure equilibrium compositions in the methane-water system at pressures to 2 kilobars in the region ambient to 350°C. Another apparatus is used to measure liquid-liquid equilibria in binary systems of water and selected hydrocarbons (such as toluene) in the region ambient to 250°C. Experimental data are correlated using semi-empirical molecular models.

Chemical Engineering Sciences

Theoretical Division
Los Alamos National Laboratory
University of California
P. O. Box 1663
Los Alamos, New Mexico 87545

Total $70,000

160. THERMOPHYSICAL PROPERTIES OF MIXTURES — 0.5 — 02-04
Jerome J. Erpenbeck

The evaluation of the thermophysical properties of mixtures of particles which interact through the hard sphere potential have been initiated using both the equilibrium techniques of Monte Carlo and molecular dynamics as well as nonequilibrium molecular dynamics. The properties under investigation are both the equations of state and transport properties, including mutual diffusion, shear and bulk viscosity and thermal conduction. These are currently under investigation at a number of densities and for several values of the diameter and mass ratio for binary mixtures. The equation of state is being compared with several approximate analytic theories, while the transport properties are compared with the Enskog theory.

Chemical Technology Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37830

Total $95,000

161. FUNDAMENTAL PROCESSES IN SORPTION PUMPING AND TRANSFER OPERATIONS USING DEEP BEDS OF SORBENTS
C. H. Byers, J. J. Perona

1.1 02-04

A fundamental framework for predicting the performance of deep-bed sorption systems is being developed for application to processes involving pumping, transfer, and storage of materials by sorption on deep beds of sorbents. Currently such techniques are utilized in a number of energy production and storage applications. An experimental program is in progress to determine the relative significance of heat and mass transfer, pressure drop, sorption equilibrium, and reaction kinetics. In the current phase, sorption processes at cryogenic temperatures in the molecular flow regime are controlled by mass transfer resistance. The assumptions used in an analytical solution to the problem are under experimental investigation in a recently reworked and expanded experimental system. Simultaneous numerical solutions are under development.

Combustion Sciences Department
Sandia National Laboratories/Livermore
Livermore, California 94550

Total $220,000

162. ANALYSIS OF REACTING, TURBULENT FLOWS
W. Ashurst, P. Barr, B. Sanders

1.5 02-04

This research consists of the development of an unsteady turbulence computational procedure for application to reacting flows with high Reynolds number and large heat release. The fluid mechanics of turbulent mixing is computed by a discrete vortex transport technique, known as Vortex Dynamics. This procedure is unique in that it relaxes some of the restrictive assumptions which must be employed in most conventional turbulence models. Current research efforts are focusing on the influence of fluid transport length and time scales on flame propagation and scalar transport in turbulent, chemically-reacting systems. Analysis of the unsteady breakup of a round fuel jet has begun. In this study the three-dimensional transport is computed near the fuel nozzle. Statistics of scalar transport and intermittency will be characterized as probability density functions for use in diffusion flame models.

OFFSITE CONTRACTS

Photochemical and Radiation Sciences

PURDUE UNIVERSITY
West Lafayette, Indiana 47907

163. STUDY OF THE MOTION OF ELECTRONS IN NON POLAR CLASSICAL LIQUIDS — $69,708 — 01-01
G. Ascarelli
Department of Physics

In our effort to study the motion of electrons injected in insulating liquids we have measured the Hall mobility of electrons injected in neopentane along the liquid gas coexistence curve between the triple point and the critical point. The time of flight mobility (TOF) has been measured on the same sample over the same range of temperatures and is in good agreement with the results found in the literature. The ratio of these mobilities is 1.8 near the triple point, decreases linearly to 1.4 near 130°C and increases again to nearly 6 at the critical point. Such a temperature dependence cannot be understood as resulting from either a combination of known scattering mechanisms or from trapping by extrinsic impurities. The large increase of the mobility ratio near the critical point suggests the influence of density fluctuations that create localized states. The leading term of the mobility calculation by Basak and Cohen, coupled with the measured value of (dV_o/dn) as well as the room temperature compressibility predicts, without any adjustable parameters, a room temperature mobility that is only 30% higher than the experimental value.

DARTMOUTH COLLEGE
Hanover, New Hampshire 03755

164. PHOTOEXCITED CHARGE PAIR ESCAPE AND RECOMBINATION — $81,539 — 24 mo. — FY 83-84 — 01-01
Charles L. Braun
Department of Chemistry

The escape and recombination of charge pairs produced by photoexcitation of organic molecules is being studied. The recombination of geminate charge pairs formed by the photoionization of solute molecules in low dielectric constant solvents is found to occur in picoseconds. This process is being studied by pump-probe conductivity techniques. Picosecond absorption measurements of the recombination kinetics are planned. The data are being compared with a detailed theory of the diffusive recombination of geminate charge pairs. The second key goal is to understand the mechanism of charge pair escape in electronically excited electron-donor-acceptor (EDA) materials. A number of donor-acceptor geometries are being explored in these solid state studies. The possible role of the lowest-energy, charge transfer (CT) state in the formation of separated charge pairs (current carriers) is of special interest. Steady-state and nanosecond pulse measurements of both photocurrents and fluorescence are being used to test mechanistic ideas.

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

165. STUDIES IN CHEMICAL REACTIVITY — $70,305 — 01-01
Robert W. Carr
Department of Chemical Engineering and Materials Science

Kinetics of elementary physical and chemical processes are being investigated by a number of experimental techniques. Flash spectroscopy and flash photolysis with time resolved mass spectrometry are being used to study the kinetics of atomic and free radical reactions in the gas phase. A flash spectroscopic study of the reaction $CF_2Cl + O_2$ has recently been completed. The collisional deactivation of highly vibrationally excited polyatomic molecules is being studied by chemical activation methods, and product analysis by gas chromatography. A photoionization method for direct detection of highly vibrationally excited molecules is being investigated. The variational method of sensitivity analysis recently developed in this laboratory is being applied to large kinetic mechanisms.

Photochemical and Radiation Sciences, continued

BOSTON UNIVERSITY
Boston, MA 02215

166. INVESTIGATIONS OF THE TRIPLET STATES OF CHLOROPHYLLS — $173,305, 24 mo., FY 83-84 — 01-01
Richard H. Clarke
Department of Chemistry

The characterization of the structures assumed by chlorophyll molecules upon aggregation in photosynthetic systems is important for an understanding of the mechanisms of energy conversion in photosynthesis. Since the properties of the excited triplet state of the pigment molecules such as the electron distribution and excited state dynamics are sensitive to the surrounding interactions and to the state of aggregation, triplet state properties serve as a convenient and nondestructive probe into the makeup of photosynthetic systems. Our present research program utilizes optical detection of magnetic resonance spectroscopy to investigate the triplet state properties of the chlorophyll molecule in lipid bilayers, in protein matrices, and as films deposited on surfaces. These measurements allow an evaluation of in vitro chlorophyll systems for structural features proposed as models for the antenna and reaction center of naturally occuring photosynthetic systems and for their general applicability as model systems for photosynthesis.

UNIVERSITY OF COLORADO/BOULDER
Boulder, Colorado 80309

167. SENSITIZING AND QUENCHING IN THE CONVERSION OF LIGHT ENERGY INTO CHEMICAL ENERGY — $61,800 — 01-01
Stanley J. Cristol
Department of Chemistry

Geometric, regiochemical and free-energy constraints for intramolecular excitation and electron transfer in bichromophoric molecules are being investigated. Factors being studied include modification of substituents present on the donor chromophore, which controls the electron-donating power of the first excited species, and the reduction potentials of the acceptor chromophores. Use of systems with rigid structures permits study of the effects of distance and geometry upon the rates of electron transfer (or the likelihood, in the case of short-lived intermediates). Work has begun on study of quantum-mechanical constraints on the electron-transfer process, that is, the question of whether electron transfer involves tunneling (electron jump) or prefers a through-bond mechanism. Substantial progress has been made in these areas.

OHIO STATE UNIVERSITY
Columbus, Ohio 43210

168. PULSE RADIOLYSIS STUDIES OF FAST REACTIONS IN MOLECULAR SYSTEMS — $75,525 — 01-01
Leon M. Dorfman
Department of Chemistry

The broad objective of this research program is to come to an understanding of the rates and mechanisms of chemical reactions induced by ionizing radiation. At the same time, the information generated about the reactive intermediates (free radicals, molecular cations and anions) is of interest in other areas of chemistry as well. Reaction is initiated by a high energy electron pulse of submicrosecond duration, and the reactive intermediates are directly observed by fast optical absorption measurement (time resolution 5 nanoseconds). These observations also provide the optical spectra of the reactive transients. Systems presently under study are: (a) organic molecular cations in solution. These ions, important in radiation-induced reactions, also play a key role in cationic polymerization. (b) Transition metal carbonyl radicals in solution, of which the absorption spectra and reactivities are determined. These free radicals play a role in homogeneous catalysis. Since the reactions are initiated by high energy electrons, the results obtained relate directly to radiation chemistry.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF CALIFORNIA/LOS ANGELES
Los Angeles, California 90024

169. TIME-RESOLVED LASER STUDIES ON THE ENERGY TRANSFER AND THE CONFIGURATIONAL CHANGES IN BACTERIORHODOPSIN — $92,000 — 01-01
M. A. El-Sayed
Department of Chemistry

Bacteriorhodopsin is another photosynthetic system besides chlorophyll. The understanding of the primary photochemical and photophysical process is of current interest. We developed time-resolved resonance Raman techniques in order to record the vibration spectra of different transients formed following the initial photosynthetic absorption process. Questions such as: a. does energy migration take place to specific sites prior to photochemistry; b. does isomerization of retinal take place on the picosecond time scale, and c) when does the Schiff base lose its proton during the photochemical cycle, are among the questions we are attempting to answer. Very recently, we started using time-resolved optical spectroscopy of the protein and the retinal systems to identify the coupling between these two systems which results in the proton pumping required for photosynthesis in bacteriorhodopsin.

STANFORD UNIVERSITY
Stanford, California 94305

170. ENERGY TRANSFER PROCESSES IN SOLAR ENERGY CONVERSION — $130,786 — 24 mo. — FY 82-83 — 01-01
M. D. Fayer
Department of Chemistry

This program is examining energy transport processes in nontraditional systems using picosecond and other optical techniques and statistical mechanical theoretical methods. There are a wide variety of situations in both natural and man-made systems which cannot be modeled as periodic arrays of molecules. In many systems inherent disorder and characteristic size and shape play key roles in determining energy dynamics. We have developed the first accurate and detailed statistical mechanics theory of energy transport in dis-ordered systems with finite volume. We are using a picosecond transient holographic grating technique and picosecond fluorescence mixing methods with conventional fluorescence and absorption experiments to study energy transport among dye molecules attached to long hydrocarbon chains organized in micelle solution, and to examine energy transport in chromophore containing polymers. These "clustered" chromophore systems permit extremely high local chromophore concentrations and therefore efficient energy transport, without the normal energy quenching associated with conventional concentrated dye solutions.

CLARKSON COLLEGE OF TECHNOLOGY
Potsdam, New York 13676

171. PHOTOCHEMICAL SOLAR ENERGY CONVERSION IN SURFACTANT VESICLES — $67,893 — 01-01
Janos H. Fendler
Department of Chemistry

Utilization of surfactant vesicles for solar energy conversion continues to be the goal of this program. The main thrust of our research has been centered upon the development of polymerized vesicles. The recognized leakage from nonpolymerized vesicles as well as lack of long term stability necessitated this approach. Polymerized vesicles are stable yet remain fluid enough to allow for proton, electron, and hydrogen permeabilities. A number of polymerizable surfactants have been synthetized. Vesicles have been formed by sonication, and characterized by steady state and dynamic laser light scattering. Vesicle polymerization has been affected by steady state irradiation or by means of chemical initiators. Vesicle sizes did not alter appreciably upon polymerization. Research has been initiated for improving the performance of hydrogen generating colloidal catalysts. Attention has been initially focused on obtaining mechanistic insight into colloid formation in the confined space of water-in-oil microemulsions and vesicles. Colloidal platinum has been stabilized in polymerized vesicles. Efforts are underway for investigating vesicle stabilized semiconductors and their use in energy conversion, electron transfer, charge separation, and water splitting.

Photochemical and Radiation Sciences, continued

OHIO STATE UNIVERSITY
Columbus, Ohio 43210

172. KINETICS OF FAST REACTIONS OF EXCITED SPECIES — $66,000 — 01-01
Richard F. Firestone
Department of Chemistry

Goals are identification of mechanisms for growth and decay of excited rare gas atoms and excimers in the presence and absence of foreign quenching agents using pulse radiolysis methods. Identities of excited atomic precursors of bound excimer states are sought by modelling of a multi-stage reversible collisional relaxation mechanism for rovibrationally excited excimer molecules in conformity with temporal behavior of excited atoms and rovibrationally relaxed excimers. Monitoring of excited species is done by emission spectrometry and tunable cw laser spectrophotometry. Kinetic parameters of selected ls-2p state pairs are to be obtained by cw pumping coupled with absorption measurements at low power densities and at power densities sufficiently great to induce bleaching of the transition.

COLUMBIA UNIVERSITY
New York, New York 10027

173. LASER ENHANCED CHEMICAL REACTION STUDIES — $155,000 24 mo. FY 82-83 — 01-01
George W. Flynn
Department of Chemistry

This project is aimed at the study of chemical reactions of laser pumped molecules with particular emphasis on the role of vibrational energy transfer processes in chemical dynamics. Fast hydrogen, chlorine, and deuterium atoms are being produced by pulsed excimer laser photolysis of gaseous diatomic molecules. These medium hot atoms cause vibrational excitation of stable molecules during collisions or react chemically to form products inaccessible to thermally cold species. Infrared fluorescence is being used to probe the broad spectral distribution of vibrationally and rotationally hot CO, CO_2, and CH_3F molecules produced in these atom-molecule encounters. An infrared laser diode is also employed to monitor, with a resolution of milliwavenumbers, the precise vibrational and rotational states excited during such collisions. Laser induced visible and U.V. fluorescence methods are being used to identify the species and to measure the distribution of final states formed as a result of chemical reaction.

UNIVERSITY OF TEXAS/AUSTIN
Austin, Texas 78712

174. ORGANIC REDOX PHOTOTRANSFORMATIONS AT CHEMICALLY MODIFIED SURFACES — $120,000 24 mo. FY 82-83 — 01-01
Marye Anne Fox
Department of Chemistry

Exploratory and mechanistic studies of new chemical transformations of organic molecules at native and chemically modified surfaces represent the goal of this research program. New electrode materials are being prepared by adsorption, covalent attachment, polymerization, and mulling with electroactive or light-sensitive materials, and physical studies of the properties of these materials are being conducted. Both photocatalytic and photosynthetic organic reactions can be initiated by electron exchange induced by visible light excitation of either native chemically modified semiconductor surfaces. Several spectroscopic techniques are being used to evaluate intermediates and surface states: Fourier transform infrared spectroscopy, Resonance Raman spectroscopy, laser-induced flash coulostatic measurements, photochemically induced magnetic resonance, picosecond laser spectroscopy, rotating ring disc electrochemical techniques, and ESCA and Auger spectroscopy. New metal non-oxides and p-type semiconductors are also being investigated and the search for new reactions on these novel materials is continuing.

Photochemical and Radiation Sciences, continued

WASHINGTON UNIVERSITY
Saint Louis, Missouri 63130

175. REACTION STUDIES OF HOT SILICON AND GERMANIUM RADICALS — $86,000 — 01-01
Peter P. Gaspar
Department of Chemistry

The goals of this research program are to discover what are the reactions of high energy Si and Ge atoms, how do the reactions take place, and how are the reaction pathways influenced by the energy and electronic state of the free atoms and of the reactive intermediates that they produce. Silicon and germanium atoms are formed at high energies by nuclear transformations such as $^{31}P(n,p)^{31}Si$ and $^{76}Ge(n,2n)^{75}Ge$, and at low energies by thermal evaporation. Intermediates such as SiH_2 and $GeMe_2$ are generated by pyrolysis and photolysis. In the past year a new silylene rearrangement, a transposition, has been shown to be mediated by alkyl and hydrogen shifts, with a disilene intermediate: $Me_3Si\text{-}Si\text{-}H \rightleftharpoons Me_2Si{=}SiMeH \rightleftharpoons Me_2HSi\text{-}Si\text{-}Me$. The ratio of transposition to intramolecular C-H insertion by the silylene has been determined as a function of temperature, and the results will permit the determination of the vibrational temperature of these intermediates when produced in recoil reactions. Rate measurements have been initiated via laser flash photolysis of the reactions of a silylene Me-Si-Ph in solution.

TEMPLE UNIVERSITY
Philadelphia, Pennsylvania 19122

176. DYNAMIC ASPECTS OF THE DYE-SENSITIZED PHOTOCONDUCTIVITY OF SEMICONDUCTORS — $66,579 — 01-01
Antonio M. F. Goncalves
Department of Chemistry

The objective of this program is to probe the dynamics of the elementary processes (injection, recombination, and escape) which determine the efficiency of dye-sensitized semiconductor/electrolyte solar cells. The general experimental approach relies primarily on the use of subnanosecond time-resolved spectroscopic techniques: fluorescence and transient absorption or gain. The fluorescence lifetimes of several dyes adsorbed on semiconductors and insulators at high surface coverage are on the order of 50 picoseconds, as much as 30 times shorter than in solution. The fact that a similar lifetime reduction occurs for each dye both on semiconductor and insulator surfaces suggests that energy transfer quenching is primarily responsible for the short lifatimes. This is confirmed by preliminary fluorescence quantum yield measurements as a function of surface coverage: In the limit of very low surface coverage the quantum yield approaches the solution value on an insulator and a much smaller value on a semiconductor. These experiments indicate that injection occurs in a time on the order of 150 ps.

UNIVERSITY OF FLORIDA
Gainesville, Florida 32611

177. RADIATION CHEMISTRY OF HYDROCARBON AND ALKYL HALIDE SYSTEMS — $65,000 — 01-01
Robert J. Hanrahan
Department of Chemistry

Current work is directed towards understanding the mechanism of product formation in the gamma and pulsed electron radiolysis of simple chemical systems. Studies of the radiolysis of hydrogen - carbon monoxide mixtures on alumina surfaces include measurement of both hydrocarbon and oxygen-containing products; certain yields are increased by 100 times or more in comparison to the gas phase. The radiolytic oxidation of propane shows many similarities to auto-oxidation in products and reaction pathways; computer modeling of the reaction scheme accounts for the oxygen pressure dependence of product yields. Measurements are being made on the rates of attack of OH radicals on hydrocarbon and halocarbon gases, using the pulse radiolysis method. Comparison of results at high and low water concentration yields data on the rates of OH + radical combination reactions in these systems. Photolysis of methyl iodide - perfluoromethyl iodide mixtures forms several products including methane and perfluoromethane, ethane and perfluoroethane, and several mixed products such as trifluoromethane, difluoroethylene, and trifluoroethane, along with HI and HF.

Photochemical and Radiation Sciences, continued

BOSTON UNIVERSITY
Boston, Massachusetts 02215

178. STUDY OF INTERMEDIATES FROM TRANSITION METAL EXCITED-STATE ELECTRON-TRANSFER REACTIONS — $70,000 — 01-01
Morton Z. Hoffman
Department of Chemistry

This research is concerned with the kinetic and mechanistic behavior of intermediates that result from excited-state electron-transfer reactions involving transition metal coordination complexes and quenchers in solution. These species are generated by means of continuous and flash photolysis or from the interaction of substrates with radiation-generated radicals using continuous and pulse radiolysis techniques. Emphasis is currently being placed on the modes of formation and decay of reduced viologens. Viologens form photoactive, luminescent charge-transfer complexes with sacrificial electron donors; the magnitude of complexation, photoreduction, and luminescence is being studied as a function of pH and solution composition. Ion-pairing and complexation have a significant effect on the quantum yield of reduced viologen when the system is photosensitized by tris-(2,2'-bipyridine)ruthenium(II) ion. In acidic solution, reduced viologens undergo hydrogenation in the presence and absence of catalytic platinum. The goal of the research is to understand the fundamental chemistry governing the generation of energy-rich charge-separated species.

OREGON GRADUATE CENTER
Beaverton, Oregon 97006

179. FUNDAMENTAL STUDIES IN CHARGE SEPARATION AT INTERFACES IN RELATION TO WATER PHOTOLYSIS — $90,000 — 16 mo. — FY 83-84 — 01-01
James K. Hurst
Department of Chemistry & Biochemical Sciences

This research is directed at improving our conceptual understanding of the influence of microphase separation and compartmentation upon photostimulated redox processes. Three distinct activities are encompassed by these studies: examination of mechanisms of transmembrane redox across bilayer membranes, development of inorganic two-photon excitation schemes for transmembrane charge separation, and development of reversed micellar assemblies for water photolysis. Redox systems under study which exhibit net electron exchange across bilayers include lecithin-bound amphiphilic 4-alkylpyridinepentaammineruthenium$^{2+/3+}$ ions and dihexadecylphosphate-bound alkylviologen$^{+/2+}$ ions. Studies in two-photon excitation are based upon photoreduction of cupric ion to cuprous π-complexes which are capable of long-range photoinitiated electron transfer to oxidant sites. In reversed micelles, the relationship between O_2 and H_2 yields and the topographic organization of Zn(II) porphyrin sensitizers, viologen charge relays and colloidal RuO_2 and Pt sols is being explored. For all photoinitiated systems, pulsed laser spectrophotometry is being used to probe reaction dynamics.

BOSTON UNIVERSITY
Boston, Massachusetts 02215

180. FORMATION OF FUEL VIA PHOTOCHEMICAL ELECTRON TRANSFER — $192,000 — 24 mo. — FY 83-84 — 01-01
Guilford Jones, II
Department of Chemistry

This research involves investigation of photochemical electron transfer reactions which are of potential utility in photoformation of fuel or useful chemicals. New reagents are under development that would permit the separation of oxidation and reduction components through temporary storage of redox equivalents in stable photoproducts. Novel sulfur heterocycles capable of two-electron oxidation are of particular interest as electron relays for experiments involving bulk solution and electrode-electrolyte interfacial electron transfer. Studies also encompass photoinduced electron transfer reactions of organic dyes which are bound to water soluble polymers. Applications of electron transfer in photochemical decomposition of hydrogen sulfide, hydrogen halide, as well as water, are under consideration.

72

Photochemical and Radiation Sciences, continued

LOUISIANA STATE UNIVERSITY
Baton Rouge, Louisiana 70803

181. THEORETICAL STUDIES OF ELECTRON AND PROTON TRANSFER PROCESSES IN FLUIDS — $40,160 — 01-01
Neil R. Kestner
Department of Chemistry

This research program is designed to study electron and proton transfer processes in fluids, especially those which could be important in energy conversion. General theoretical studies are probing the role of temperature, pressure, and solvent effects on electron transfer rates. Our special attention is directed to such effects for reactions in the "abnormal" or highly exothermic regions. Related work is exploring structure-activity relations which are important in the related proton transfer processes. The general theories are being applied to specific reactions. In this regard we are determining very accurate water-water interactions and other intermolecular potentials, exploring in detail the role of basis set errors. These are being used to obtain accurate interaction energies between electron transfer species such as Fe(II) and Fe(III) in aqueous solutions. Other studies are directed at predicting electron transfer rates in glasses and highly viscous media.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF HOUSTON
Houston, Texas 77004

182. CHARGE SEPARATION IN PHOTOREDOX REACTIONS — $160,000 — 01-01
Larry Kevan — 24 mo.
Department of Chemistry — FY 82-83

The objective of this research is to probe the molecular mechanistic and structural aspects of charge separation in photoredox reactions in micellar and vesicle systems in order to eventually couple this charge separation to chemical energy storage. Tetramethylbenzidine (TMB) has been photoionized to produce the cation radical in liquid and frozen micellar solutions of anionic, cationic and nonionic surfactants and in liquid and frozen synthetic, anionic and cationic vesicle solutions. The cation is observed by optical absorption, electron spin resonance and electron spin echo spectrometry. Cation-water interactions have been detected by electron spin echo modulation analysis and indicate stronger interactions in micellar compared to vesicular solutions. The photoproduced cation is deduced to be located asymmetrically within both the micellar and vesicular structures. Optical spectra of TMB in micellar and vesicular solutions indicate stronger hydrogen bonding interactions to TMB in the micellar solutions. Specifically deuterated surfactant molecules are being developed to better locate the photoproduced cations within these systems.

THE UNIVERSITY OF ALABAMA
Tuscaloosa, Alabama 35486

183. ELDOR INVESTIGATIONS OF RADIATION PROCESSES — $62,711 — 01-01
Lowell D. Kispert
Department of Chemistry

The objective of this research is to determine how a crystalline lattice affects energy transfer and primary radiation and photochemical processes in irradiated organic crystals. Such information is vital to understanding photoinduced solid-state polymerization, electron transport, and stereospecific reactions in solids. Electron spin resonance, electron-nuclear double resonance and electron-electron double resonance spectroscopy are being used to identify the molecular fragments formed and to detect the energy transfer processes that occur. In particular, selected sugar, polyalcohol, carboxylic acid, and acetamide crystals are being studied to determine the effect of hydrogen bonding on radical stability and reaction mechanisms as a function of temperature in crystals containing (a) varying crystallographic forms, (b) rotational disorder, and (c) impurities. Preexisting electron traps, first observed by this research, are being studied in crystals of rhamnose and trehalose, radical intermediates have been identified in irradiated β-carotene and halogenated acetamide anions have been detected.

Photochemical and Radiation Sciences, continued

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

184. STUDIES IN SPECTROSCOPY AND CHEMICAL DYNAMICS — $88,000 — 01-01
Aron Kuppermann
Division of Chemistry and
Chemical Engineering

Studies are being conducted on two color laser spectroscopy. The experiments consist of exciting a molecule with one laser and then, with a second laser time-delayed with respect to the first one, inducing either a downward transition or an additional excitation. The downward transition permits the study of highly vibrationally excited states of the ground electronic state (stimulated emission pumping) and the additional excitation permits the investigation of the dynamics properties of electronically excited states. These studies are aimed at understanding the properties of highly excited vibrational and/or electronic states of molecules. Studies are also being conducted using variable angle electron impact spectroscopy to investigate spin forbidden electronic transitions in stable molecules and beams of free radicals. These transitions are difficult to induce by other means and the states produced play important roles in photochemistry, radiation chemistry, electric discharge chemistry and plasma chemistry.

PENNSYLVANIA STATE UNIVERSITY
University Park, Pennsylvania 16802

185. THE FREE-RADICAL AND ION CHEMISTRY OF VOLATILE SILANES, GERMANES AND PHOSPHINES — $127,270 — 01-01
F. W. Lampe
Department of Chemistry

This research program consists of experimental studies of the chemical reactions initiated by the irradiation of gaseous silanes, germanes and phosphines with ionizing radiation, infrared laser radiation and vacuum-ultraviolet light. From the experimental studies fundamental reaction mechanisms relative to this new and unexplored chemistry are developed. In particular, the knowledge and understanding developed enables us to attempt useful exploitations of photochemical and radiation chemical techniques for the synthesis of amorphous solids of silicon, germanium, phosphine and mixtures thereof. Presently under study is the infrared laser photochemistry of SiH_4-HCl and SiH_4-PH_3 mixtures, CH_3SiH_3, the vacuum-ultraviolet photochemistry of GeH_4 and GeH_4-NO mixtures, and the ion chemistry of SiH_4-CH_3Cl, SiH_4-CH_2Cl_2, and GeH_4-C_2H_4 mixtures.

BROWN UNIVERSITY
Providence, Rhode Island 02912

186. A UNIFIED APPROACH TO CHARACTERIZATION OF COLLISIONS BETWEEN REACTIVE RADICAL PAIRS IN SOLUTION — $60,000 — 01-01
Ronald G. Lawler
Department of Chemistry

A program is underway to systematically characterize the reactive and unreactive encounters between simple organic free radicals in aqueous and organic solvents. Three general techniques are being employed: (A) kinetics of bimolecular radical decay as measured by EPR, (B) measurement of bimolecular contributions, especially Heisenberg spin exchange, to electron relaxation times, and (C) determination of enhancement factors for chemically induced magnetic polarization (CIDNP and CIDEP). Radicals are generated at present primarily by pulse electron radiolysis of aqueous solutions of simple organic acids and alcohols using facilities at Argonne National Laboratory. Studies are being extended to organic solvents using peroxides as radical precursors and employing NMR and EPR detected laser flash photolysis. Theoretical models are being developed both to extract data from rapidly varying magnetic resonance spectra detected by pulsed methods and to interpret (A)-(C) in terms of molecular properties of the radicals and the medium in which they react.

Photochemical and Radiation Sciences, continued

NATIONAL BUREAU OF STANDARDS
Washington, D.C. 20234

187. SUPPORT OF CRITICAL DATA COMPILATIONS — $200,000 — 01-01
David R. Lide, Jr.
Office of Standard Reference Data

The Office of Standard Reference Data of the National Bureau of Standards administers a collaborative interagency program for the preparation of compilations of physical and chemical reference data. Current projects within the scope of the Division of Chemical Sciences fall in the following areas: physical and thermodynamic properties of fluids, solubility, electrolyte properties, atomic data relevant to fusion, and thermodynamics of high-temperature systems. The approach is to review critically all relevant data from the literature, compare with theory, and select the most reliable values. Whenever possible, correlations are developed which allow prediction of unmeasured properties. Reviews are in press on high-temperature vaporization of alkali metal oxides, water solubility of polynuclear aromatic compounds, electrochemical equilibria in carbon-oxygen systems, and other topics.

WAYNE STATE UNIVERSITY
Detroit, Michigan 48202

188. ELECTRONIC RELAXATION PROCESSES IN POLYATOMIC MOLECULES — $76,330 — 01-01
Edward C. Lim
Department of Chemistry

The purpose of this research is to gain fundamental understanding of radiationless transitions in exciplexes and charge-transfer complexes, which are pertinent to photochemical energy conversion. Both the steady-state and time-resolved measurements of fluorescence and triplet formation are employed to study factors which influence various nonradiative decay channels in condensed phase. The results indicate that the dominant nonradiative decay channel of these species at moderately high temperatures (room temperature and above) may be internal conversion to the ground state. They also suggest that there is a propensity rule for singlet-triplet intersystem crossing in charge-transfer complexes. Thus, singlet-triplet intersystem crossing from a charge-transfer singlet state appears to be efficient only when a locally excited triplet state of a component molecule (donor or acceptor) lies below the charge-transfer singlet state, consistent with vanishingly small spin-orbit coupling between charge-transfer states.

BRANDEIS UNIVERSITY
Waltham, Massachusetts 02254

189. PHOTOCHEMICAL REACTIONS OF COMPLEX MOLECULES IN CONDENSED PHASE — $90,000 — 01-01
Henry Linschitz
Department of Chemistry

The main purpose of this program is the identification and evaluation of factors governing the efficiency of primary radical formation in photochemical redox reactions. This is a general problem in photochemical energy conversion since charge-transfer kinetic intermediates may lead either to radical products or dissipative quenching. Reaction rates and quantum yields are measured by laser flash photolysis on redox systems including particularly porphyrins or anthraquinones, with inorganic anions as donors. The sharp increase in yield with anion concentration is attributable to changes in spin-orbit coupling within the primary reaction complex. Studies on covalently-linked porphyrin-quinone systems of known geometrical configuration are in progress to determine effects of donor-acceptor distance and orientation. Other research is concerned with photo-isomerization of dipyrrylmethenes and shifts in proton-transfer equilibria accompanying formation of rotational conformers.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

190. THE CONTRIBUTION OF ELECTRONICALLY EXCITED STATES TO THE RADIATION CHEMISTRY OF ORGANIC SYSTEMS
Sanford Lipsky
Department of Chemistry
$180,000
24 mo.
FY 82-83
01-01

A general study is being made of those photophysical properties of organic molecules that have relevance in determining their radiation-chemical behavior. Projects currently in progress include: (a) A study of the dependence on scavenger concentration of the efficiency of quenching geminate-ion recombination fluorescence of saturated hydrocarbon liquids in order to characterize the distribution function of electron-positive ion separation distances. (b) A study of the dependence on photon energy of the probability of photoionization and of the average range of the electron ejected from aromatic solutes in non-polar fluids via comparison with theory of the effect of an electric field to reduce the geminate-ion recombination fluorescence. (c) A study of the effect of perfluorocarbons to alter the distribution function of electron-positive ion separation distances by interaction with epithermal electrons as manifested by an altered electric field dependence of photocurrent.

DREXEL UNIVERSITY
Philadelphia, Pennsylvania 19104

191. A STUDY OF PHOTOSENSITIZED REDOX REACTIONS IN MICROEMULSIONS
Raymond A. Mackay
Department of Chemistry
$55,000
01-01

The objective of this research program is to explore the utility of microemulsions as media for solar energy conversion systems. An evaluation of the effect of sensitizer and reductant location in the microdroplet is being made by measuring the quantum yield of the photoreduction of methyl red by either ascorbate or hydrazobenzene in the presence of various surfactant porphyrin sensitizers. The mechanism of the enhancement, with respect to water, of the power output of a surfactant thionine-iron (II) thin layer photogalvanic cell employing an anionic microemulsion as the solvent is being investigated by means of flash photolysis and conventional spectroscopy. The use of auxiliary sensitizers in such photogalvanic cells is being concurrently examined by means of both steady-state irradiation experiments and energy transfer studies. The latter are being carried out in the very optically dense solutions required for effective cell operation.

UNIVERSITY OF NEBRASKA
Lincoln, Nebraska 68588

192. ENERGETICS OF THE FORMATION AND REACTIONS OF GASEOUS IONS
G. G. Meisels
Department of Chemistry
$90,000
01-01

Two areas are addressed. One uses threshold photoelectron-coincidant photoion mass spectrometry to study ions whose internal energies are known within 0.025 meV. The energetics of the formation, isomerization and fragmentation of ions are measured. Nitromethane and nitrobenzene ions have activation barriers and rearrange before fragmentation. Modifications to allow study of collision processes are underway. The other area correlates ion residence times with the point of ionization by impact of 100 to 600 eV electrons. Linear ionization rates are highest at the point of entry and decrease smoothly with penetration. Ranges are derived; they are near the higher limits calculated by theoretical models, suggesting that the measured quantity lies between the real range and the electron path length.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF NORTH CAROLINA / CHAPEL HILL
Chapel Hill, North Carolina 27514

193. ENERGY CONVERSION PROCESSES BASED ON MOLECULAR EXCITED STATES — $98,000 — 01-01
Thomas J. Meyer
Department of Chemistry

The research effort is based on the study and exploitation of excited states of transition metal complexes. A particularly important goal is the design and characterization of new classes of photosensitizers and their application to solar energy related problems. In technical detail the work involves the measurement of the photochemical and photophysical properties of excited states, the application of theory to such processes, synthesis of new types of potential photosensitizers, the preparations and properties of metallopolymers containing metal complex chromophores, the study of electron and energy transfer processes of the photosensitizers in solutions and polymeric films, and possible applications of these materials in photochemical and photoelectrochemical energy conversion processes.

NATIONAL BUREAU OF STANDARDS
Washington, DC 20234

194. PULSE RADIOLYTIC STUDIES OF INTER- AND INTRAMOLECULAR ELECTRON TRANSFER PROCESSES — $125,000 — 01-01
P. Neta, S.G. Liss, M. Mautner
Center for Chemical Physics

Studies of both intermolecular and intramolecular electron transfer processes are conducted using pulsed electron sources to generate the reactive intermediates, and time resolved absorption spectrophotometry to follow the kinetics of the ensuing reactions. Quantitative results are obtained detailing the effects on the rates of intramolecular electron transfer of the charge distribution within the molecule, electron affinities of substituents, steric effects, and other structural parameters. Intramolecular electron transfer reactions within metalloporphyrins are also studied because of the importance of these molecules in photosynthesis and because they allow a detailed analysis of the effect of driving force and other parameters on the rates of these processes. The mechanism and thermodynamics of intermolecular electron transfer reactions are studied using measurements of rate and equilibrium constants as a function of temperature to obtain quantitative information about activation energies, enthalpy and entropy changes associated with these processes. Comparison of values of liquid and gas phase systems will permit a more quantitative understanding of solvation effects in electron transfer processes.

CLEMSON UNIVERSITY
Clemson, South Carolina 29631

195. INTRAMOLECULAR ENERGY TRANSFER REACTIONS AS A METHOD FOR METAL COMPLEX ASSISTED PRODUCTION OF HYDROGEN — $110,000 24 mo. Fy 82-83 — 01-01
John D. Petersen
Department of Chemistry

The current research effort concentrates on coupling highly absorbing metal centers to potentially photoactive metal centers (e.g., metal dihydrides) by covalent bonding through bridging ligands. This is done in order to use low energy light to drive useful chemical reactions by intramolecular energy transfer processes. Major emphasis has been on bridging ligands that will chelate both metal centers, and form short, highly-conjugated links between the metal centers. One of these bridges, 2,2'-bipyrimidine (bpym) has been used to link a series of metal centers together to form a metallopolymer with the formula $[Ru(bpym)Cl_2]x(bpym)$, which is black in color and has two potential derivative sites on each metal center.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF NEBRASKA
Lincoln, Nebraska 68588-0304

196. HIGH ENERGY HALOGEN REACTIONS ACTIVATED BY NUCLEAR TRANSFORMATIONS — $65,000 — 01-01
Edward P. Rack
Department of Chemistry

The fundamental goal of this project is to understand better the chemical reactivity of high energy monovalent species. High energy reactions of halogen atoms or ions activated by nuclear transformations are studied in gaseous, high pressure and condensed phase saturated and unsaturated hydrocarbons, halomethanes and liquid and solid aqueous solutions of biological molecules. Specifically, the stereochemistry involving single chiral center molecules, systematics, mechanisms and halogen reactivity in a collapsing molecular environment and caging of halogen hot atoms in an ice lattice are under investigation. The stereochemistry of exothermic halogen atom homolytic bimolecular substitution (S_H2) at the chiral centers of chiral 2-halopropionyl halides is currently studied. Practical applications of recoil atom chemistry to activation analysis for trace elements or molecules in biological or environmental systems, to radiopharmacy involving synthesis and radioprotection, and to the study of solute-solute and solute-solvent interactions of dilute aqueous solutions of biological molecules are being carried out.

CARNEGIE-MELLON UNIVERSITY
Pittsburgh, Pennsylvania 15213

197. SOLAR ENERGY CONVERSION IN HOMOGENEOUS SOLUTION — $60,427 — 01-01
Robert M. Richman
Department of Chemistry

The goal of this project is to study the photochemistry of compounds that are likely to photodisproportionate. This mechanism has the potential for doing useful oxidations and reductions without the need for a non-dissociative long-lived charge transfer excited state. Irradiation of μ-oxo-bis((tetraphenylporphinato)-iron(III)) at $\lambda < 440$ nm yields the ferryl ion, FeOTPP. Irradiation with sunlight of a cyclohexene solution results in catalytic oxidation to cyclohexene-2-one with several thousand turnovers. Inclusion of thallium (III) benzoate may yield the epoxide. Flash photolysis allows direct observation of the transient FeOTPP. Analogous photochemistry is observed with $(FeTPP)_2N$ and $(FeTPP)_2C$. Use of charged porphyrins allows study in aqueous solution and may increase quantum yield by lowering back reaction rates. Irradiation in the presence of CoTPP may yield the novel mixed-metal FeTPP-O-CoTPP. Irradiation of $[Ru(NH_3)_5]_2O^{4+}$ results in substitution followed by reduction.

UNIVERSITY OF CALIFORNIA/DAVIS
Davis, California 95616

198. NUCLEAR METHODS IN CHEMICAL KINETICS — $48,000 — 01-01
John W. Root
Department of Chemistry

This research program is designed to probe the chemical reactions of atomic fluorine. These reactions are initiated by recoiling radioactive fluorine-18 atoms produced using cyclotron induced nuclear reactions. The measured data include the distributions and the relative rates of formation of the labeled reaction products at sample pressures ranging from 0.1 to 200 atmospheres. The derived results include the mechanisms of product formation, the internal excitation energy distributions, and the unimolecular decomposition and collisional energy transfer behavior of the nascent species formed in hot halogen-for-hydrogen and halogen-for-halogen atomic exchange reactions. With simple fluorocarbons, these reactions probe center-of-mass collision energies in the range from ca. 2 to more than 25 eV. In the presence of excess inert moderator, these techniques also allow kinetic measurements to be performed for the reactions of thermal fluorine-18 atoms. Studies of this type are in progress with simple organic reagents.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, California 92717

199. RESEARCH IN CHEMICAL KINETICS — $170,000 — 01-01
F. S. Rowland
Department of Chemistry

This research program is directed toward the understanding of the rates and mechanisms of chemical reactions, including some of interest to atmospheric chemistry. The reactions of thermalized ^{18}F and ^{38}Cl atoms with gaseous $(CH_2{=}CHCH_2)M$ compounds are being studied for M=Sn, Ge, Si, C to determine the extent of restricted intramolecular energy flow ("non-RRKM") in such systems. Reactions of halogen atoms with haloolefins (X + $CH_2{=}CHY$; X=F,Cl; Y=F,Cl,Br) are furnishing rate information about radical lifetimes, and mechanistic information such as selectivity and isomerization. The temperature dependence of ^{38}Cl reactions with olefins is being studied over the 240-360 K temperature range. The mechanism of the direct gas-phase photolysis of $^{14}CS_2$ is being investigated with and without O_2 present. The rates and mechanisms of hydrolysis in aqueous solution are being measured for gases occurring in the atmosphere, including OCS, CH_3I and CH_3Br. The gas phase photolyses of PH_3 and P_2H_4 and the co-photolysis of PH_3 and NH_3 are being investigated. The possibility of hot Cl abstraction by energetic ^{38}Cl atoms is being tested.

WORCESTER POLYTECHNIC INSTITUTE
Worcester, Massachusetts 01609

200. THE GAS PHASE RADIOLYSIS AND VACUUM ULTRAVIOLET PHOTOLYSIS OF HETEROCYCLIC ORGANIC COMPOUNDS — $43,000 — 01-01
Alfred A Scala
Department of Chemistry

The objective of these studies is to gain a better understanding of how complex organic molecules react when they absorb the high energies characteristic of γ-radiolyses and vacuum ultraviolet photolyses. Emphasis is being placed on the reactions of heterocyclic compounds containing oxygen, nitrogen or sulfur. Since ions as well as neutrals are produced in these systems the rate constants for related ion-molecule reactions are being measured by photoionization mass spectrometry. This work has been extended to include chemical ionization at pressures in the vicinity of one atmosphere. This is an effort to produce even-electron ions of the type important in solution phase organic chemistry in order to facilitate evaluation of the role of the solvent in organic chemistry.

CHARLES F. KETTERING RESEARCH LABORATORY
Yellow Springs, Ohio 45387

201. PARTICULATE MODELS OF PHOTOSYNTHESIS — $65,000 — 01-01
Gilbert R. Seely

The program consists of the investigation of photophysical and photochemical properties of chlorophyll, absorbed together with other amphiphilic molecules on particles of polyethylene swollen with low molecular weight hydrocarbon diluents. When suspended in aqueous media, the particles are intended to provide a viscous medium for anchorage of the hydrophobic parts of amphiphilic molecules. In general, chlorophyll is maintained in monomeric form in the presence of amphiphiles that interact with it, such as alkylamides, or as fluorescent dimers or higher aggregates at greater concentration. Specific aspects under investigation include absorption, fluorescence, and CD spectroscopy, energy transfer among chlorophyll species, and photochemistry. With regard to the last, the behavior of particles with chlorophyll and oxidizing amphiphilic ligands is receiving particular attention.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF PUERTO RICO/MAYAGUEZ
Mayaguez, Puerto Rico 00708

202. PHOTOELECTROCHEMISTRY OF NEW PHENOTHIAZINE DYE DERIVATIVES — $125,000, 24 mo., FY 83-84 — 01-01
Fernando A. Souto
Department of Chemistry

This program has been designed to study the potential of amphiphilic derivatives of thionine for a better understanding of photochemical energy conversion with aqueous systems in solution. The main objective is to investigate the kinetics associated with their photoreduction with ferrous ions. The work carried out thus far has consisted of the synthesis and the preliminary characterization of derivatives that are disulfonated, dimethyldisulfonated, trisulfonated, and with other groups. The uv-vis spectra of these dyes are similar to that of thionine (599 nm) with maxima in the range 570-625 nm, but with the exception that there is no evidence for wasteful self association at conc. c.a. 10^{-3}M. The solubility of the disulfonated thionines is about 10^{-2}M in 0.1N H_2SO_4 (thionine c.a. 5.10^{-5}M). The extinction and diffusion coefficients change with the nature and position of substituents on the thiazine nucleus, but no clear effects can yet be realized. The rate constants for the back reaction between the leucothiazines and ferric ion are all faster than the value of thionine, with one exception which merits further characterization. Work is in progress to further test these compounds in the presence of micellar assemblies.

UNIVERSITY OF UTAH
Salt Lake City, Utah 84112

203. DYNAMICS AND MECHANISMS OF CATALYTIC PROCESSES AND HOT CHEMISTRY — $100,000 — 01-01
Leonard D. Spicer
Department of Chemistry

This research is designed to investigate reaction kinetics and mechanisms, collision dynamics, and energy transfer in thermal, photochemical, and hot reactions. Electronic excitation with and without photochemical rearrangement of active catalyst species is used to study the critical transition state for processes involving Wilkinson's catalyst and to generate new metal centered catalytic molecules. The kinetics of the photochemical processes are being modeled and include the formation of a new isomerization catalyst having a half life of several minutes. The active catalytic species is postulated to be a fluxional molecule having adjacent olefin and η^3-allyl ligands. Nuclear recoil chemistry is being used to study hot reaction dynamics. The recoil distribution for chlorine atoms from the $^{35}Cl(n,\gamma)^{36}Cl$ process is being determined from the reported prompt gamma ray spectrum. The cooling characteristics of recoil tritium atoms at high moderation in the presence of reactive hydrocarbons are also being modeled. The new material, ammonium trimethylsilylsulfite, from this laboratory is being tested as a standard for solid state NMR.

PRINCETON UNIVERSITY
Princeton, New Jersey 08544

204. PHOTOELECTROCHEMISTRY WITH CHEMICALLY MODIFIED ELECTRODES — $80,300 — 01-01
Thomas G. Spiro
Department of Chemistry

The electrochemistry and photoelectrochemistry of metalloporphyrin electrode films is being explored, with a view toward catalyzing useful energy storage reactions, including the splitting of water to H_2O_2. Stable metalloprotoporphyrin films have been prepared via electroinitiated polymerization of the vinyl side-chains, and other porphyrin polymerization schemes are being explored. Cobalt porphyrins are being applied to the catalysis of H_2 production from water, while iron, chromium and manganese porphyrins are being explored in oxidative chemistry, with the eventual aim of catalyzing water oxidation.

Photochemical and Radiation Sciences, continued

MOUNT HOLYOKE COLLEGE
South Hadley, Massachusetts 01075

205.	PHOTOELECTROCHEMISTRY OF ORGANIC DYES Mark T. Spitler Department of Chemistry	$114,000 24 mo. FY 82-83	01-01

The oxidation of organic dyes adsorbed at semiconductor surfaces is being studied through photoelectrochemical techniques to determine the role of electron transfer in the quenching of the excited state of the dye. The utilization of an attenuated total reflection method enables an in situ determination of the quantum efficiency of current producing photoreactions at both metal and semiconductor surfaces. Photooxidation of dyes at ZnO, TiO_2, and $SrTiO_3$ single crystal surfaces is being investigated using dyes that show significant triplet character or tendency to form aggregates. Estimation of the degree of excitation quenching caused by this oxidation is also obtained through concomitant measurements of the fluorescence intensity of the adsorbed dye. The photoassisted oxidation of triphenylmethane dyes at Au and Pt electrodes is also being studied using an internal reflection technique which permits spectral characterization of reaction products.

UNIVERSITY OF ARIZONA/TUCSON
Tucson, Arizona 85721

206.	MECHANISMS OF PHOTOCHEMICAL ENERGY CONVERSION BY CHLOROPHYLL Gordon Tollin Department of Biochemistry	$160,627 24 mo. FY 83-84	01-01

The goals of this project are to elucidate the detailed mechanisms involved in light-induced one-electron transfer reactions involving chlorophyll (and related compounds) and electron donors and acceptors, and to determine the interactions between the elementary steps in these processes and environmental parameters such as viscosity, dielectric constant and homogenous vs. heterogeneous reaction matrices. The intent is to develop a body of fundamental information which can be used to devise strategies for increasing the yields of the high energy products of such reactions, to physically separate these products and to decrease the probability of recombination (i.e. back reaction), and to facilitate secondary electron transfer to external donors and acceptors. Current work involves the use of laser flash photolysis to monitor excited state and radical dynamics in lipid bilayer vesicle systems.

81

Photochemical & Radiation Sciences, continued

UNIVERSITY OF MASSACHUSETTS AT BOSTON
Boston, Massachusetts 02125

207. INVESTIGATION OF THE STRUCTURE OF PHOTOSYNTHETIC REACTION CENTERS — $66,451 — 01-01
Hans van Willigen
Department of Chemistry

The research program concerns the study of the structure of photosynthetic reaction centers and model systems with the aid of magnetic resonance techniques. Measurements of the electron spin distribution in the photoexcited triplet state of these systems with the aid of Electron Spin Resonance (ESR) and Electron Nuclear Double Resonance (ENDOR) are used to obtain structural information. Research has focused on the ENDOR measurement of hyperfine interactions in the photoexcited triplets of a series of porphyrins. Also, the study has been concerned with the application of ESR and ENDOR in the study of aggregate formation of a number of water-soluble porphyrins. These systems are of interest because of their use as photo catalysts for the water splitting reaction $2\ H_2O \rightarrow 2\ H_2 + O_2$. Furthermore, they constitute ideal model systems for the investigation of the effects of aggregation on the photophysics and photochemistry of porphyrins.

UNIVERSITY OF ILLINOIS/CHICAGO
Chicago, Illinois 60680

208. EVALUATION OF THE ESE ENVELOPE MODULATION TECHNIQUE FOR STUDIES OF FREE RADICALS — $38,000 — 01-01
Robert I. Walter
Department of Chemistry

Analysis of the electron spin echo envelope modulation (ESEEM) can give precise information on the hyperfine parameters for dilute crystals of paramagnetic species. The objective of this work is to determine whether the method can also yield useful data on free radicals in random glassy solution, the only state in which some important biological samples can be prepared and observed. A series of nitroxide radicals which differ in deuterium labelling or in structural constraints on geometry, and three other nitrogen-centered radicals selected for small ^{14}N coupling constants (in the range 2.1 to 7.6 gauss) have been prepared. These radicals are examined in a random glassy matrix by the three-pulse electron spin echo technique; this part of the research is carried out at the Argonne National Laboratory under the supervision of James Norris. The ESEEM results are not consistent with the working hypothesis that small hyperfine coupling constants should appear in the spin echo modulation. Instead, the nuclear quadrupole moment of ^{2}D or ^{14}N dominates the echo modulation, and should be the major source of information about samples studied by this technique.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, California 93106

209. ENERGY TRANSFORMATIONS IN TRANSITION METAL COMPLEXES — $82,863 — 01-01
Richard J. Watts
Department of Chemistry

The projects in this program are intended to explore basic photochemical and photophysical phenomena in transition metal complexes. Five primary areas of endeavor include: 1) Photochemical and photophysical consequences of metal-carbon bonding to acceptor ligands with extended π-systems; 2) Electronic relaxation phenomena between excited states of metal complexes; 3) Mechanisms of excited state electron transfer reactions; 4) Tuning of electronic excited states by extension of π-conjugation in N-heterocyclic ligand metal complexes; and 5) Photochemistry and photophysics of organometallic sandwich complexes. The primary techniques being applied in these projects include time-resolved emission spectroscopy, laser-induced transient and excited state absorption spectroscopy, and ^{1}H and ^{13}C nmr spectroscopy. Laser double resonance techniques are presently being developed for the purpose of characterizing electronic relaxation between excited states of metal complexes. Synthesis and characterizations of complexes containing metal-carbon bonds are being carried out in order to facilitate the projects in area 1) above.

UNIVERSITY OF NORTH CAROLINA/CHAPEL HILL
Chapel Hill, North Carolina 27514

210. APPLICATIONS OF PHOTOINDUCED ELECTRON TRANSFER AND HYDROGEN ABSTRACTION PROCESSES TO CHEMICAL AND ELECTROCHEMICAL CONVERSION PROCESSES — $76,445 — 01-01
David G. Whitten
Department of Chemistry

This research program involves studies of photochemical redox reactions occurring via electron transfer and hydrogen atom abstraction processes initiated by excitation of chromophores absorbing visible and near ultraviolet light. A part of the project involves direct study of photochemical reactions and external factors which can modify them. In addition, photoelectrochemical processes based on them are being investigated. Our studies of direct photochemical reactions have recently focused on photoredox reactions of certain indigo dyes. It develops that these dyes undergo net photoreduction processes with a variety of electron donors by, in some cases, a multiplicity of mechanisms. Among the most interesting mechanisms are a net hydride ion transfer which occurs via a sequence of electron, proton, and second electron transfer, all within the initially formed encounter complex. We are also investigating the effect of inclusion complex formation on reactivity using various amylose derivatives as selective hosts for a variety of reactive substrates. The photoelectrochemical studies are currently focusing on hydrogen atom abstraction reactions from alcohols occurring with substrates excited by visible light.

UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

211. STUDIES IN HOT ATOM AND RADIATION CHEMISTRY — $21,019 — 24 mo. — FY 82-83 — 01-01
J. E. Willard
Department of Chemistry

The objectives of this continuing project are to obtain a better understanding of the production, migration, trapping, reactions and spectra of free radicals, hydrogen atoms, electrons, and ions formed in solid organic matrices at 4 K - 200 K. The species studied are formed by irradiation with γ-rays, X-rays, and ultraviolet radiation. Electron spin resonance, ultraviolet, visible and infrared spectrometry are used for analysis. Current emphasis is on the investigation of hydrogen atoms, free radicals and mercury adducts formed by mercury photosensitized decomposition of CH_4 in CH_4 and rare gas matrices; and the role of neutralization processes in radical production in radiolyzed hydrocarbons.

Photochemical and Radiation Sciences, continued

UNIVERSITY OF TENNESSEE
Knoxville, Tennessee 37996

212. STUDIES OF RADIATION-PRODUCED RADICALS AND RADICAL IONS — $92,000 — 01-01
T. Ffrancon Williams
Department of Chemistry

The basic objective of this program is to characterize important free radical and radical ion intermediates generated by irradiation of molecular systems. Current emphasis is being placed on the radical ions produced in the primary chemical processes resulting from the absorption of high energy radiation. Novel radical ions derived from typical saturated molecules are being generated and stabilized in suitable solid matrices, examples being fluorocarbon radical anions in hydrocarbon matrices and the radical cations of alkanes, ethers, and organometals of Group IVB alkyls in fluorocarbon matrices. Electron spin resonance (ESR) spectroscopy is used to identify these paramagnetic species. Measurements of hyperfine coupling constants, including those of ^{13}C-labeled radicals, provide information about geometrical structure and spin density distribution. The chemical rearrangement of positive ions is also being investigated. Studies are also underway on the generation and characterization of organometallic radicals and radical ions in systems which are relevant to catalysis and solar energy conversion.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts 02139

213. PHOTOCHEMICAL ENERGY STORAGE: STUDIES OF INORGANIC PHOTOASSISTANCE AGENTS — $245,000 — 01-01
Mark S. Wrighton
Department of Chemistry

Light-driven, energy-storing chemical reactions are the object of study in this research program. Emphasis is on the use of semiconductor electrodes as the photoassistance agents for redox reactions such as the oxidation and reduction of H_2O. Fundamental studies of the nature of semiconductor/electrolyte interfaces to establish the energetics and kinetics for light-driven redox processes are one aspect of the program. Semiconductor materials under study in this connection include WS_2, InP, GaAs, Si, CdX (X=S, Se, Te), and amorphous hydrogenated Si. Another aspect of the program is chemical derivatization of the semiconductor surface for the purpose of improving durability and kinetics for the desired redox reaction. In the area of electrocatalysis surface modification with metals, oxides, and polymers is being studied. Catalysis of halide oxidation and H_2O reduction have received most attention. Exploratory studies to find unique interactions of redox reagents with semiconductor electrode surfaces, such as I_3^-/I^- with n-WS_2, are in progress. Such unique interactions are likely to lead to high efficiency for energy conversion and specific redox processes.

Chemical Physics

CORNELL UNIVERSITY
Ithaca, New York 14853

214. SHOCK TUBE PYROLYSIS OF AROMATIC HYDROCARBONS -- DETECTION OF SOOT PRECURSORS — $52,142 — 01-02
Simon H. Bauer
Department of Chemistry

The objectives of the shock tube experiments are to determine the fragmentation patterns for structurally related di- and tri-cyclic aromatics, to measure the relative levels of soot produced, and to formulate semi-quantitative mechanisms for these processes. The experiments are performed in a single-pulse shock-tube with a coaxial laser beam absorption diagnostic. Gas chromatographic analyses are made of samples extracted from the downstream end of the shock tube. During the test time attainable with this configuration (700-900 μs) the quenched samples are kinetically limited. The shapes of the He/Ne transmission curves indicate that the attenuation of the beam is not due to loss by scattering from the final product but to absorption by precursor species, the concentrations of which first rise and then decline due to subsequent reactions. This technique presents a possibility for recording their extended absorption spectra.

THE UNIVERSITY OF CHICAGO
Chicago, Illinois 60637

215. TOPICS IN FINITE TIME THERMODYNAMICS — $70,000 — 01-02
R. Stephen Berry
Department of Chemistry and the James Franck Institute

The term "finite time thermodynamics" refers to the extension of traditional thermodynamics to the description of systems and processes whose constraints include finite times or nonzero rates of operation. In particular, the term refers to the determination of the extremal performance and the paths that would yield that performance, when the constraints of finite-time operation must be met. The recent progress of this group has included: the theoretical description of a new type of engine, based on a dissipative process; an analysis of heat engines subject to periodic boundary conditions (as with the diurnal variations of solar systems); the exploration of geometric formulation of thermodynamics based on the metric introduced by Weinhold; a first study of separation processes, involving an analysis of the use of multiple points of heat exchange in distillation columns as a means of minimizing the production of excess entropy, and finally, the extension of the concept of availability (exergy) to processes operating in finite time, and the application of this extended concept to extraction of work from a system not initially in internal equilibrium.

COLUMBIA UNIVERSITY
New York,NY 10027

216. ENERGY PARTITIONING IN ELEMENTARY GAS PHASE REACTIONS — $35,000 — 01-02
Richard Bersohn
Department of Chemistry

The dynamics of the elementary reactions A + BC $\rightarrow$ AB + C and A + BCD $\rightarrow$ AB + CD are being studied by a two laser experiment. One laser generates the reactive atoms A (carbon, hydrogen, fluorine or sulfur) by photodissociation of a suitable parent molecule. The second laser probes the internal state distribution of the products. Reactions studied include: $S(^1D)$ + OCS and F + RI where R=H, CH_3, C_2H_5, i-C_3H_7 and t-C_4H_9. For all R the abstraction product IF was probed and for R = CH_3 and C_2H_5 the iodine atom product of the Walden inversion was also found. Spectroscopic techniques are being developed for studying the time dependence of atomic concentrations, in particular of different atomic sublevels.

Chemical Physics, continued

ILLINOIS INSTITUTE OF TECHNOLOGY
Chicago, Illinois 60616

217. THEORETICAL STUDIES OF COMBUSTION DYNAMICS — $59,000 — 01-02
Joel M. Bowman
Department of Chemistry

The objective of this research is to develop and apply approximate but accurate quantum mechanical methods to reactions of interest in gas phase combustion. Such a theory has been developed and applied to the reactions $O(^3P) + H_2$, $O + D_2$ and $O + HD$ using an accurate ab initio potential energy surface. Extension of the theory to treat diatom + diatom reactions has been made and the first application will be to the $OH + H_2$ reaction. A surface will be obtained from new ab initio calculations that are planned by Dr. Thom Dunning. Work is also underway to calculate the vibrational energies and lifetimes of HCO and HOCO using an ab initio potential surfaces calculated by Harding. This work is based on a vibrational self-consistent field plus configuration interaction method developed here. The interaction of radiation with long-lived collision complexes is also being investigated and preliminary calculations indicate that stabilization by stimulated emission may be feasible for small systems using lasers of moderate power.

YALE UNIVERSITY
New Haven, Connecticut 06520

218. SIMULTANEOUS MULTIPOINT MEASUREMENTS OF DENSITY GRADIENTS AND TEMPERATURE IN A FLAME — $63,000 — 01-02
R. K. Chang (Applied Physics), B. T. Chu and M. B. Long (Mechanical Engineering)

Research is currently under way to develop and apply new optical diagnostic techniques to the characterization of turbulent reacting flows. Spontaneous Raman scattering is being used to map out the fuel gas concentration at 2500 points within a plane intersecting the flow in a single laser pulse (1.8 μsec). For this type of "Ramanography" experiment, a high-energy single-pulse laser system is required. A further requirement of the laser is that the peak power not be so high as to cause breakdown of the gases when the beam is focused. While this type of laser is not readily available commercially, the Diana dye laser available at the Combustion Research Facility (CRF) at Sandia National Laboratories in Livermore, California has the unique characteristics needed for this work. Experiments are therefore being carried out at the CRF and preliminary results demonstrate the feasibility of the technique. The ability of the technique to give the instantaneous fuel gas concentration distribution at many points within a plane is important for studying the interaction of the turbulence with the chemistry in these complex flows.

UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

219. UNIMOLECULAR DECAY DYNAMICS — $44,524 — 6 mo. — 01-02
F. Fleming Crim
Department of Chemistry

This program is an experimental study of the unimolecular decay dynamics of internal energy selected molecules using direct production of highly vibrationally excited molecules by dye laser excitation of overtone vibrations in conjunction with time resolved spectroscopic detection. Recent experiments determine the product quantum state distributions in the unimolecular decay of hydrogen peroxide (HOOH) and its partially deuterated analogue (HOOD) excited to the fifth overtone ($v = 6$) of the OH stretching vibration. These measurements also provide spectra of overtone vibrations which reveal rotational structure and combination transitions. The product state distributions appear to differ qualitatively for excitation of a combination transition compared to excitation of a pure stretching vibration. Statistical (phase space) calculations describe the essential features of the product state distributions except for the case of excitation of a combination band. This experimental technique is providing uniquely detailed data on the unimolecular reaction dynamics of selectively excited molecules.

Chemical Physics, continued

SRI INTERNATIONAL
Menlo Park, California 94025

220. COMBUSTION RESEARCH PROGRAM: FLAME STUDIES, LASER DIAGNOSTICS AND CHEMICAL KINETICS — $109,000 — 01-02
David R. Crosley
Molecular Physics Laboratory

This research program involves a combination of laser-induced fluorescence (LIF) and chemical kinetics measurements to investigate the chemistry of combustion processes. The research comprises several related parts: LIF probing of flat flames, the development of an LIF spectroscopic and collisional data base, computer modeling of combustion chemical networks, development and application of rate constant estimation methods, and a laser pyrolysis (LP)/LIF experiment. In the LP/LIF technique, reactants are rapidly heated through absorption (by SF_6 seeded in the mixture) of pulsed CO_2 laser radiation, with LIF measurements of radical concentrations and temperature made as a function of time. The LP heating processes and the test reaction OH + CH_4 have been investigated over the range 800-1400 K. Measurements of the rate constant for OH + C_2H_2 at 1200 K show an abstraction mechanism, in contrast to the addition channel which dominates at room temperature. In a flow system, the laser spectroscopy of the $A^3\Pi_i - X^3\Sigma^-$ system of NH has been studied, yielding lifetime, quenching, and transition probability information.

WILLIAM MARSH RICE UNIVERSITY
Houston, Texas 77251

221. INFRARED ABSORPTION SPECTROSCOPY WITH COLOR CENTER LASERS — $61,000 — 01-02
Robert F. Curl
Department of Chemistry

This research program is directed at the development of high sensitivity, high resolution methods for detecting and monitoring small free radical species which are thought to be important intermediates in combustion by means of infrared absorption spectroscopy using color center laser sources. A magnetic rotation technique for the suppression of source noise combined with the long pathlengths obtainable with a White cell provides a high sensitivity absorption spectroscopy which is selective for free radicals. With this arrangement, the electronic spectrum of C_2H in a discharge through argon over polyacetylene, has been observed and assigned. The Ballik-Ramsay bands of C_2 have also been identified in this system. In the continuation of this work, efforts will focus upon the identification of other radical species present in the discharge over polyacetylene and the search for new radical spectra (CH_2, CH_2OH, HCCN, and N_2H_3). In addition, the development of a new high sensitivity spectroscopic method suitable for non-magnetic molecules using electro-optic tone modulation of the color center laser infrared output will be pursued.

PRINCETON UNIVERSITY
Princeton, New Jersey 08544

222. COMPREHENSIVE MECHANISM FOR THE COMBUSTION CHEMISTRY OF ALCOHOLS: AN EXPERIMENTAL & NUMERICAL STUDY WITH EMPHASIS ON APPLIED SENSITIVITY ANALYSIS — $79,117 — 01-02
Frederick L. Dryer
Dept. of Mech. and Aero. Engineering

With the exception of methanol, alcohols have received little attention with regard to mechanistic description of actual combustion chemistry. The current work addresses the development of a comprehensive detailed kinetic model for the pyrolysis and oxidation of ethanol. Intermediate temperature (ca. 1000 K) turbulent flow reactor data at atmospheric pressure are obtained to provide initial insights as to the phenomenology of these reactions, and these data are combined with higher temperature results (shock tubes, flames) in developing a detailed mechanism. Acetaldehyde appears as a major intermediate in this mechanism, and thus the work also provides a comprehensive pyrolysis and oxidation mechanism for this species. The mechanism development itself as well as the property behavior of the result are studied using the sensitivity analysis techniques developed by Rabitz and co-workers at Princeton.

Chemical Physics, continued

UNIVERSITY OF COLORADO
Boulder, Colorado 80309

223. LASER PHOTOELECTRON SPECTROSCOPY OF IONS — $57,000 — 01-02
G. Barney Ellison
Department of Chemistry

Laser photoelectron spectroscopy has been used to study a number of simple negative ions. Our experiments produ direct, reliable thermodynamic information such as electron affinities, radical and ion heats of formation, and bond dissociation energies. These are crucial data required for an understanding of combustion processes. We have completed careful studies of HNO^-, DNO^-, CH_2CCH^-, CH_2CCD^-, CD_2CCH^-, CCO^-, $HCCO^-$ and $DCCO^-$. We have finished work on CH_2CN^-, CD_2CN^-, CH_2NC^-, and CH_3CHCN^-. Proposed research centers on polymeric carbon ions (C_n^-), allyl anion (CH_2=CH-CH_2^-), and CO_2^-.

UNIVERSITY OF OREGON
Eugene, Oregon 97403

224. LASER SPECTROSCOPY OF COMBUSTION INTERMEDIATES — $28,500 — 01-02
Paul Engelking
Department of Chemistry

Molecular radicals important to combustion chemistry are being investigated by electronic spectroscopy. Besides providing wavelengths of optical transitions for practical use in the laser probing of flames and combustion environments, this research obtains basic information concerning the structure, the relative energies of electronic states, and the internal dynamics and reactivities of radical species. Current investigation includes a spectroscopic search for the lowest electronic state of CH, analogous to the newly discovered first excited state of CF, and an investigation of the spectroscopy of CH_3N. These species have been implicated in the fixation of nitrogen by flames.

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

225. LASER-INDUCED ORGANIC REACTIONS IN THE GROUND ELECTRONIC STATE — $54,000 18 mo. FY 83-84 — 01-02
William E. Farneth
Department of Chemistry

This project is an investigation of the potential and present utility of high power infrared and visible lasers for initiating and directing chemical reactions of organic molecules. Laser-induced chemical reactions in both homogeneous gas phase systems and in heterogeneous gas/solid mixtures have been examined. The work attempts to define strategies for using the spatial, temporal or energetic resolution of the laser activation step to influence the rate and selectivity of subsequent chemical reactions. Specific systems investigated include: cyclopropane and oxacyclobutane derivatives with IR excitation, alcohols in the presence of CuO with IR excitation, and t-butylhydroperoxide with visible excitation. In the alcohol/CuO chemistry, for example, laser variables and system variables can be used to alter the ratio of dehydration to dehydrogenation from essentially exclusive dehydration in the homogeneous system to predominant dehydrogenation under certain heterogeneous conditions.

Chemical Physics, continued

UNIVERSITY OF ROCHESTER
Rochester, New York 14627

226. LOW ENERGY ION-MOLECULE REACTIONS AND CHEMIIONIZATION KINETICS — $65,000 — 01-02

James M. Farrar
Department of Chemistry

Molecular beam reactive scattering measurements of proton transfer reactions of the flame cations HCO^+ and H_3O^+ with neutral molecules present in hydrocarbon flames are being carried out to understand the dynamics of ionic processes occurring in flames. Measurements of product angular and kinetic energy distributions yield energy disposal in reactive collisions, inferences concerning preferred collision geometries, and in favorable cases, determination of specific quantum states of nascent reaction products. Proton transfer reactions to the substrates H_2O, CH_3OH, C_2H_5OH, and $(CH_3)_2C{=}O$ have been studied, indicating direct reaction dynamics. Unimolecular decay channels of protonated products are studied and decays involving bond cleavage, 1,3-hydrogen atom shifts, and elimination of molecular hydrogen across the C-O bond have been observed. In the latter case, variation of proton donor modifies the parent ion internal state distribution; such observations are being employed to assess the role of tunneling through the exit channel barrier in the elimination process. Work in progress involves hydride transfer reactions of CH_3^+.

AEROCHEM RESEARCH LABORATORIES, INC.
Princeton, New Jersey 08540

227. EXPERIMENTAL DETERMINATION OF RATE COEFFICIENTS FOR IMPORTANT COMBUSTION/FUEL CONVERSION REACTIONS BY A NOVEL HIGH-TEMPERATURE PHOTOLYSIS TECHNIQUE — $70,673 — 01-02

William Felder

The aim of this project is to measure the temperature-dependent rate coefficients for isolated, elementary reactions important in fossil fuel combustion and pollution processes. The flash photolysis/resonance fluorescence or absorption technique is used for rate coefficient measurements. The temperature range of this technique was extended in this work to permit measurements from room temperature (300 K) to practical combustion temperatures (up to 1800 K). Current work emphasizes reactions of OH radicals produced in the flash photolysis of water. Preliminary results for reaction of OH with benzene and methane yield $k(OH + C_6H_6) = (3.0 \pm 0.8) \times 10^{-11} \exp[-(2.32 \pm 0.30) \times 10^3/T]$ cm^3 molecule^{-1} s^{-1} (840-1370 K) and $k(OH + CH_4) = (5.5 \pm 1.6) \times 10^{-11} \exp[-(2.9 \pm 0.36) \times 10^3/T]$ cm^3 molecule^{-1} s^{-1} (970-1460 K). The first direct rate coefficient measurements on the reaction $H + H_2O \rightarrow OH + H_2$ were made above 1100 K. Our work shows that this reaction can interfere in any kinetic study on OH above ca. 1000 K if H_2O is used as a precursor. We obtain $k(H + H_2O) = (5.2 \pm 4.5) \times 10^{-19} \exp[-(11.2 \pm 1.1) \times 10^3/T]$ cm^3 molecule^{-1} s^{-1} (1160-1390 K). Measurements at higher temperatures for these OH reactions are in progress.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, New York 12181

228. KINETIC MEASUREMENTS ON ELEMENTARY FOSSIL FUEL COMBUSTION REACTIONS OVER WIDE TEMPERATURE RANGES — $80,000 — 01-02

Arthur Fontijn, Department of Chemical and Environmental Engineering

This, recently initiated, research program is aimed at providing kinetic data on important isolated elementary hydrocarbon molecule oxidation reactions. Emphasis is placed on measurements in the 1000-1800 K range, where accurate data are generally not available, but needed for development of improved fossil-fuel utilization methods. The high-temperature photochemistry (HTP) adaptation of the flash-photolysis resonance-fluorescense technique is further developed. Use is made of fast electronics, which allows rapid data taking and short residence times, and of on-line microcomputer data smoothing procedures which minimize the number of flashes required. The first objects for study are reactions between O atoms and C_2 hydrocarbons.

Chemical Physics, continued

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

229. STATE-TO-STATE DYNAMICS OF MOLECULAR ENERGY TRANSFER — $75,000 — 01-02
W.R. Gentry and C.F. Giese
Departments of Chemistry and Physics

A novel pulsed molecular beam instrument has been constructed for the study of state-to-state vibrational and rotational energy transfer in collisions of atoms and molecules. The results are expected to lead to an understanding of molecular energy transfer on a microscopic level, including the dependence of energy transfer processes on the vibrational and translational energies of the colliding molecules. The first experiments measured the kinetic energy dependence of the vibrational excitation cross sections for I_2 + He collisions. Similar measurements have now been performed for I_2 + D_2 and I_2 + Ne collisions, in order to explore the effects of mass and features of the potential energy surface on the excitation dynamics. These experiments are being extended to other systems, including mode-specific excitation of polyatomic molecules.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

230. REACTION MECHANISMS IN COMBUSTION: FORMATION OF SOOT AND POLYCYCLIC AROMATIC HYDROCARBONS — $70,000 — 01-02
William A. Goddard III
Department of Chemistry

We are examining the microscopic mechanisms of the gas phase and heterogeneous processes involved in the formation of soot and of polycyclic aromatic hydrocarbons during combustion. The emphasis this year has been on the development of methods for describing the dynamics of the heterogeneous processes involved in the growth of the soot particle. This has led to the Classical Stochastic Diffusion Theory in which the classical dynamical equations of motion are transformed to a generalized Langevin equation (involving explicitly only those atoms of the surface directly bonded to the adsorbate) which is solved by taking the Markovian limit appropriate to the long time scale for the growth processes. Detailed comparison of these first principles rate predictions with experimental rates for desorption shows excellent agreement.

UNIVERSITY OF ILLINOIS/CHICAGO
Chicago, Illinois 60680

231. KINETICS OF ELEMENTARY ATOM AND RADICAL REACTIONS — $66,357 — 01-02
Robert J. Gordon
Department of Chemistry

The objectives of this research are to measure the reaction rates and to study the dynamics of elementary gas phase reactions, using sensitive, real time techniques to eliminate systematic errors. One system being studied is O+H_2, D_2 and HD. Measurements of the O+H_2 rate constant at 470K, using flash photolysis with resonance fluorescence detection of O atoms, show that previous values of the rate constant were 2-4 times too high. Accurate measurements of the rate constants for all three isotopes are being performed at temperatures up to 1000K. The intramolecular branching ratio for O+HD is being determined by using laser-induced fluorescence to measure the relative concentrations of OH and OD products. In a separate study the relaxation of highly excited molecules is being studied by using a CO_2 laser to excite a "donor" molecule while detecting IR fluorescence from a "receptor" molecule. Studies of SF_6 + H_2O and SF_6 + NO yield the VV transfer rate as a function of SF_6 excitation. The observation of a slower decay rate at higher excitation levels indicates the existence of an energy storage mechanism in the SF_6 molecule.

90

Chemical Physics, continued

BROWN UNIVERSITY
Providence, Rhode Island 02912

232. INTERACTIONS OF MOLECULES WITH SURFACES — $65,000 — 01-02
E.F. Greene
Department of Chemistry

The rate of desorption of Cs,K,Na and Li atoms from the (100) and (111) surfaces of silicon is followed by surface ionization. The rates are markedly lower from surfaces stable in the temperature range 800-950K than they are from metastable ones supercooled below surface phase transitions. These are the well-known one for (111) at 1120±40K and one for (100) at 980±20K. On the metastable surfaces the desorption is first order and the atoms appear to be highly mobile. On the stable surface where the desorption is mixed first and second order the atoms are also highly mobile but concentrated at steps between terraces from which most of the desorption occurs. In a different experiment molecules of tetramethyldioxetane are given kinetic energy by being seeded into nozzle beams of hydrogen. This kinetic energy is converted by a single collision with a surface into internal energy of the molecules which then can decompose and emit light. The amount of light varies with the kinetic energy, the temperature of nozzle, and the nature of the surface. This experiment offers an effective method of activating the decomposition of gaseous molecules.

UNIVERSITY OF UTAH
Salt Lake City, Utah 84112

233. THE STUDY OF COMBUSTION AND FLAME PROCESSES INITIATED BY IR LASER-INDUCED ABSORPTION — $114,000 — 01-02
William A. Guillory
Department of Chemistry

The phenomenon of infrared multiple-photon absorption (IR MPD), subsequently leading to excited and ground state dissociation products, simulates non-equilibrium processes occurring in flames and other combustion systems. Using visible and UV laser-induced fluorescence diagnostics as probes of the reaction zone, highly sensitive time and wavelength resolved spectroscopy allow detailed determination of the mechanisms and energetics of a given system. The reactions of vibrationally excited ground electronic state CH and OH (produced by IR MPD) with O_2, N_2, NO and aliphatic and aromatic hydrocarbons are being studied. Also being studied is the efficiency and means of production, via IR MPD, of CH and OH from various precursors. New techniques, such as multi-photon absorption fluorescence, are being implemented to study amounts of and energy states of reactive and product species (CH_2, CH_3, CO, etc.). Discrete level and quasicontinuum energy transfer and relaxation in propynal, glyoxal and methylglyoxal are also being studied.

ILLINOIS INSTITUTE OF TECHNOLOGY
Chicago, Illinois 60616

234. STUDIES OF COMBUSTION KINETICS AND MECHANISMS — $110,000 — 01-02
David Gutman
Department of Chemistry

The purpose of the research is to gain new quantitative knowledge of the kinetics and mechanisms of the reactions of polyatomic free radicals which are important in hydrocarbon combustion processes. The free radicals are generated in a heated tubular reaction by the multiple-photon-induced decomposition of suitable precursors by a CO_2 TEA laser. The ensuing reactions are monitored using a photoionization mass spectrometer capable of recording the time evolution of either reactants or products. The recombination of C_2H_5 radicals are being studied in detail. Special procedures to determine their initial concentrations are also being developed. The reactions of alkyl radicals with molecules are being investigated as a function of pressure as well as temperature. In particular the $C_2H_5+O_2$ reaction is being studied from 300-1000K and from 0.4 to 8 torr total pressure. Details of mechanism changes at elevated temperatures are being obtained.

Chemical Physics, continued

STANFORD UNIVERSITY
Stanford, California 94305

235. COMBUSTION GAS SPECTROSCOPY USING TUNABLE LASERS — $33,000, 6 mo. — 01-02
R. K. Hanson
Department of Mechanical Engineering

Objectives of this research are: (1) the measurement of fundamental spectroscopic parameters (absorption coefficients, band or oscillator strengths and collision widths) for critical combustion species, particularly pollutants and radicals; and (2) the development of tunable laser absorption techniques for species measurements in studies of chemical kinetics. Laser sources include a tunable CW infrared diode laser, a tunable CW ring dye laser and a discretely tunable CO laser. Species currently under study include HCN, CO, OH, C_2H_2, H_2O, NH, CH, NCO and CH_3. Measurements are made over a range of conditions in a controlled-temperature absorption cell, in the post-flame region of a flat flame burner and in a shock tube.

STANFORD UNIVERSITY
Stanford, California 94305

236. THE KINETICS OF SOME REACTIONS OF HCN AT HIGH TEMPERATURE — $65,000 — 01-02
Ronald K. Hanson and Craig T. Bowman
Department of Mechanical Engineering

The objective of this research program is to obtain high-temperature kinetic data for reactions involving HCN and the CN radical. These data are relevant to the formulation of reaction mechanisms for pollutant formation in flames. Reactions of interest include the thermal decomposition of HCN, the reactions of HCN with CN, H, O and OH, the thermal decomposition of C_2N_2 and the reactions of CN with O and O_2. A conventional shock tube technique is combined with spectroscopic diagnostics to study the mechanisms and rates of candidate reactions. Experimental data are compared with results obtained from empirical models.

HOWARD UNIVERSITY
Washington, District of Columbia 20059

237. LASER STUDIES OF THE DYNAMICS OF ATOM MOLECULE REACTION — $50,000 — 01-02
William M. Jackson
Department of Chemistry

This program has been designed to use tunable dye lasers to measure reaction rates of CN free radicals as a function of their internal energy. The project is based upon unique photochemical sources of internally excited CN radicals that can be produced from the laser photolysis of C_2N_2, ClCN and BrCN. Each of these respective compounds produce CN radicals that are rotationally or vibrationally hot. The amount of rotational and vibrational excitation depends upon the compound used so that by measuring the rate constant as a function of particular source of CN, we hope to be able to obtain information about the effects of internal excitation on the rate constants for CN reaction.

Chemical Physics, continued

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

238. HIGH RESOLUTION INFRARED SPECTROSCOPY: DYNAMICS OF VIBRATIONALLY EXCITED STATES — $64,000 — 01-02
Kenneth C. Janda
Department of Chemistry

Molecular beam laser photodissociation spectroscopy is used to characterize intramolecular energy redistribution in excited vibrational states of molecules. Van der Waals molecules are used as prototypes for this effect because deposition of one infra-red photon is enough to break a bond. The goal is to have a description of the interim molecular energy transfer in microscopic detail. It appears that vibrational predissociation of triatomic molecules is well described by Fermi's golden rule perturbation theory. This theory predicts that a HeI_2 molecule would have short-lived vibrationally excited states, 10^{-10} sec., while the $NeCl_2$ molecule would have long-lived vibrationally excited states, greater than 10^{-5} sec. This dramatic dependence of predissociation lifetime on molecular structure has now been observed. For larger molecules simple theories do not seem to apply. For example, a series of constituents were bound to ethylene. The series included Ne, Ar, HF, HCl, NO, C_2H_4. In spite of the broad distribution of molecular structures and binding energies in this series, the vibrational predissociation lifetimes are all on the picosec. timescale.

STATE UNIVERSITY OF NEW YORK/STONY BROOK
Stony Brook, New York 11794

239. MULTIPHOTON DISSOCIATION SPECTROSCOPY AND PHOTOCHEMISTRY OF TRANSIENT SPECIES — $74,357 — 01-02
Philip M. Johnson
Department of Chemistry

In order to investigate the characteristics of the photochemistry of mixed clusters of hydrocarbons and oxidants such as oxygen and nitrous oxide formed in a supersonic expansion, benzene and nitrous oxide or oxygen have been expanded together in around 20 atm of helium, resulting in large clusters containing up to around thirty benzene molecules and an indeterminate number of oxidant molecules. When irradiated with the 249 nm light from a KrF laser, the resulting mass spectrum contains only parent and fragments containing carbon and hydrogen. Upon 193 nm irradiation, however, masses are seen corresponding to inclusion of one to four oxygen atoms. In experiments to examine whether the oxidation products are the result of an ionic reaction or have a neutral precursor, a 193 nm pulse was used to irradiate the clusters initially. This photolytic pulse was followed by an ionizing probe pulse (249 nm) after a delay of up to 100 μsec. Even after this long time there is a substantial product containing oxygen, showing that either it or a precursor are stable neutral species.

UNIVERSITY OF NEW ORLEANS
New Orleans, Louisiana 70148

240. IDENTIFICATION AND TEMPORAL BEHAVIOR OF RADICAL INTERMEDIATES FORMED DURING THE COMBUSTION AND PYROLYSIS OF GASEOUS FUELS — $55,000 — 01-02
Ralph D. Kern, Jr.
Department of Chemistry

The practical and environmentally acceptable use of fossil fuels containing aromatic hydrocarbons in furnaces and engines is dependent upon the control of soot formation. The chemical sequence of reactions which lead to soot are being investigated by recording the product profiles generated during the pyrolyses of toluene, benzene, allene, butadiene, and acetylene. The experimental technique utilized involves the dynamic sampling of the reflected shock zone by time-of-flight mass spectrometry. Data have been obtained over a wide range of temperature and fuel concentrations. Computer modeling has successfully fit many of the experimental profiles. The major findings are the dominance of the ring fragmentation routes as opposed to ring condensation steps in the pyrolyses of toluene and benzene, the limited amount of ring formation observed in the decompositions of allene and butadiene, and the absence of ring species formed during the polymerization of acetylene.

Chemical Physics, continued

UNIVERSITY OF ILLINOIS/CHICAGO
Chicago, Illinois 60680

241. LASER SCHLIEREN, SHOCK TUBE STUDIES OF HIGH TEMPERATURE HYDROCARBON PYROLYSIS RATES — $61,000 — 01-02
John H. Kiefer
Department of Chemical Engineering

This project investigates the rates and mechanisms of fuel pyrolysis reactions of importance in combustion at very high temperatures. Experiments use the shock tube in conjunction with laser-schlieren diagnostics capable of providing an accurate measure of initiation rates with 0.1 μs resolution as well as some secondary rates. Rates and mechanisms for the pyrolysis of propane, propene, ethane, ethylene/acetylene, and butadiene have been investigated. The ethane study strongly indicates that methyl-methyl reactions, other than recombination, do not occur at significant rates to 2700K. The butadiene study suggests a "low" heat of formation for vinyl radical ($\Delta H_{f,298}^{\circ} < 65$ kcal/mole), and an estimate for the high-T vinyl radical dissociation rate, a rate of considerable importance in combustion modeling.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts 02139

242. DEPOPULATION RATES FOR COMBUSTION-RELATED SPECIES IN LONG-LIVED (↑>100μs) VIBRATIONALLY OR ELECTRONICALLY EXCITED LEVELS — $106,000 — 01-02
James L. Kinsey and Robert W. Field
Department of Chemistry

In this project, a new technique called Stimulated Emission Pumping (SEP) is being used to study individual levels of polyatomic molecules with chemically significant amounts (up to ~3.5eV) of vibrational excitation. Current effort focusses on the acetylene molecule, HCCH, in its electronic ground state ($\tilde{X}^1\Sigma_g^+$). Individual rotation-vibration levels as much as 28000 cm^{-1} above the vibrationless level are being studied to obtain information about the transition from regular to chaotic behavior in a molecular system. Parallel investigations are probing triplet levels of acetylene at ~45000 cm^{-1}, using Zeeman quantum beat spectroscopy and anticrossing spectroscopy. Among other things, these studies address the location of the HCCH→H+C_2H dissociation limit from the variation of the density of triplet levels.

THE JOHNS HOPKINS UNIVERSITY
Baltimore, Maryland 21218

243. IONIC ASPECTS OF SOOT FORMATION — $64,983 — 01-02
Walter S. Koski
Department of Chemistry

Two classes of ion-molecule reactions frequently cited as pertinent to soot formation are being investigated in our laboratory. The first includes proton transfer reactions from HCO^+ and H_3O^+. The variation of cross section as a function of projectile energy is being studied for the reactions $HCO^+(H_2O,CO)H_3O^+$, $HCO^+(C_6H_6,CO)C_6H_7^+$, $D_3O^+(C_6H_6,D_2O)C_6H_6D^+$ and between D_3O^+ and napthalene. The second class of reactions being examined are condensation reactions. In examining the reaction of $C_2H_2^+$ with C_2H_2 the condensation product, $C_4H_4^+$, is observed in binary collisions as are the ions $C_4H_3^+$ and $C_4H_2^+$. Examination of the kinetic energy spectra of these products shows that the ion $C_4H_3^+$ results from the decomposition of $C_4H_4^+$. On the other hand, the ion $C_4H_2^+$ arises from a more direct process. In examining the reaction of $C_2H_3^+$ with C_2H_2, no condensation product ($C_4H_5^+$) is observed although this ion ($C_4H_5^+$) is observed in the mass spectra of flames. Other ionic products from this reaction, $C_4H_3^+$ and $C_4H_2^+$ are observed with small cross section. Similar results are being observed for C_6 products arising from the reaction of $C_4H_3^+$ and C_2H_2.

Chemical Physics, continued

STATE UNIVERSITY OF NEW YORK AT BUFFALO
Amherst, New York 14226

244. MULTIPHOTON INTERACTIONS IN MOLECULES WITH PICOSECOND LASER PULSES — $61,800 — 01-02
Hoi-Sing Kwok
Department of Electrical and Computer Engineering

High power ultrashort CO_2 laser pulses are employed in this research program to study the multiphoton interaction behavior of polyatomic molecules. During the past year, multiphoton induced fluorescence in SO_2 was studied. Unimolecular decomposition of CF_3Br was also investigated in the presence of HI. Strong fluorescence was observed in both cases. Signals were observed with both 100 ns and 5 ns pulses. However, it was found that more energy was needed in our present laser system to extend the measurements to the low pressure/picosecond regime. Extensive modifications have been carried out to further this goal. A new plasma triggering device was invented. It makes use of a novel pin-resistor spark gap that produces photo-ionizing UV photons in large quantities. This device may have applications in UV spectroscopy. Also a silicon detector was explored as a monitoring device for the CO_2 laser. Techniques for generating high peak power (>500 MW) picosecond laser pulses are being pursued. Among them are high pressure (>10 atm) amplification and mode-locking. Semiconductor switching is also explored as a convenient method of producing picosecond laser pulses.

PURDUE UNIVERSITY
West Lafayette, Indiana 47907

245. MEASUREMENT OF RADICAL SPECIES CONCENTRATIONS AND POLYCYCLIC AROMATIC HYDROCARBONS IN FLAMES BY FLUORESCENCE AND ABSORPTION USING A TUNABLE DYE LASER — $88,000 — 01-02
N.M. Laurendeau and D.W. Sweeney
School of Mechanical Engineering

New quantitative laser fluorescence techniques are being developed to measure flame radical and polycyclic aromatic hydrocarbon (PAH) concentrations. During the past year we have (1) demonstrated OH concentration measurements using laser-saturated fluorescence and the balanced cross-rate model at atmospheric pressure under stoichiometric, fuel-rich, and sooting conditions; (2) extended this saturated fluorescence technique to the NH radical; (3) developed a linear fluorescence technique for determining PAH concentrations in a vapor mixture; and (4) made the first reported fluorescence measurements of atomic hydrogen in flames using two-photon absorption. Current research includes (1) laser-saturated OH measurements, (2) development of a quantitative model relating measured fluorescence intensity to atomic species concentration, and (3) PAH measurements at flame conditions.

UNIVERSITY OF COLORADO
Boulder, Colorado 80309

246. TIME-RESOLVED STUDIES OF FREE RADICALS AND LASER-INITIATED CHAIN REACTIONS — $65,000 — 01-02
Stephen R. Leone
Department of Chemistry and Joint Institute for Laboratory Astrophysics

Time and wavelength-resolved infrared emission techniques are used to study free radical production and reactions. Infrared emission spectra have been obtained and analyzed for combusting mixtures of low-pressure chlorine with hydrocarbons. A method has been developed to measure the absolute rate coefficients of methyl radical reactions with molecules such as chlorine and bromine. Intramolecular vibrational relaxation processes have been observed in the ground electronic state of hydrocarbons by exciting the first CH overtones and detecting the reduction in emission from these states. A multiple vibrational state analysis has been developed and applied to the extraction of rate information for very slow chain reactions.

Chemical Physics, continued

Kansas State University
Manhattan, Kansas 66506

247. DIFFUSION FLAME STUDIES OF THE CHEMICAL AND PHYSICAL MECHANISMS OF SOOT FORMATION FROM AROMATIC AND SUBSTITUTED AROMATIC FUELS, T.W. Lester, J.F. Merklin, C.N. Sorensen, Depts. of Nuc. Eng . & Physics — $56,000 — 01-02

This research program is intended to study the physical mechanisms and attendant chemistry that lead to the formation of large soot aggregates in flames. This past year, photon correlation spectroscopy (PCS) has been used to measure the diffusion constant of aerosol particles in flames. The soot aerosol data all lie in the transition Knudsen number regime, where the empirically based, Cunningham corrected Stokes-Einstein diffusion constant has been used commonly. However, the data all deviate from the theory by an order of magnitude. Possible errors in our interpretation of the experiment or experimental effects have been considered. These include, particulate polydispersity, various phoeretic effects, turbulence, and particulate change. None of these effects can explain the discrepancy. Rather the discrepancy may be due to a fundamental misunderstanding of particulate diffusion in gases when Kn > 0. Possible explanations we are currently considering include: experimental time scales compared to kinetic equilibrium time scales, correlated motion and velocity autocorrelation function long time tail effects, and particle-gas molecule interactions.

UNIVERSITY OF ARIZONA
Tucson, Arizona 85721

248. EXPERIMENTAL STUDIES OF THE IONIZATIONS AND BONDING OF SMALL MOLECULES ATTACHED TO TRANSITION METALS
Dennis L. Lichtenberger
Department of Chemistry — $35,000 6 mo. — 01-02

This research project focuses on <u>experimental</u> investigation of the electronic mechanisms of bond activation of small molecules by transition metals. The primary experimental technique is gas-phase photoelectron spectroscopy, utilizing HeI, HeII, and X-ray excitation sources. Breakthroughs have been made with the HeI source in observing detailed vibrational structure in metal ionizations. An improved HeII source design has proven to be especially valuable in understanding the valence ionizations or organometallic molecules. Gas phase core photoelectron spectroscopy has also been developed and has shown important correlations between core and valence ionizations shifts. The systems receiving most attention involve metal interactions with small organic species that are proposed intermediates in water-gas shift and Fischer-Tropsch catalysis, such as alkyls, alkenes, alkynes, methylenes, and vinylidenes. An important new study involves investigation of metal-alkyl complexes that represent intermediate stages of carbon-hydrogen bond breaking and formation.

UNIVERSITY OF CHICAGO
Chicago, Illinois 60637

249. LASER INDUCED CHEMICAL REACTIONS AND LASER-COLLISION PROCESSES
John C. Light
James Franck Institute and
Department of Chemistry — $65,000 — 01-02

Laser induced chemical processes of several types have been observed experimentally. Our research program is to develop theoretical methods to examine such processes and to permit accurate prediction of their dynamics. Methods to do exact (3-D) quantum calculations of single photon photodissociation of triatomic molecules have been developed and applied to I_2^+ and HCN using model excited state potential energy surfaces. A new representation of the problem (discrete variable representation) simplifies the calculation considerably by taking advantage of the initial localized configuration of the molecule. Similar techniques are useful in the problem of dissociative attachment of an electron to a diatomic or triatomic molecule. For the problem of multiphoton dissociation of small polyatomic molecules a new transformation and approximation (rotating frame transformation) have been developed in order to follow the time evolution of the molecular system as it gains energy from the laser field. The technique is simple and accurate enough to permit the *ab initio* calculation of the dynamics of molecules such as O_3 in strong laser fields.

Chemical Physics, continued

UNIVERSITY OF KANSAS
Lawrence, Kansas 66045

250. MOLECULAR DESIGN PRINCIPLES FOR BIOMIMETIC SOLAR ENERGY CONVERSION SYSTEMS — $84,207 — 01-02
Gerald M. Maggiora
Departments of Chemistry & Biochemistry

Ab initio quantum mechanical and empirical potential function procedures are being applied in an investigation of the physico-chemical factors underlying biological and biomimetic solar energy conversion, and these factors will be used to develop a set of molecular design principles which will enable chemists to formulate structures of potential biomimetic photoconversion systems possessing specified properties, more efficiently. Current studies are directed towards porphyrin dimer and trimer systems, especially hetero-dimers. Preliminary results indicate the existence of low-lying, non-radiative charge-transfer states in magnesium porphine-porphine dimers which may be sufficiently long-lived to facilitate electron transfer from these dimers to appropriate acceptors. The results are being further evaluated with regard to the effect of intermolecular geometry and microenvironment on the location and character of the charge-transfer states. Studies are also continuing on the evaluation of possible molecular candidates for the P700 and P680 photoactive species in the photoreaction centers of green plants. In addition, the development of new and improved theoretical methodologies and algorithms are being actively pursued.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, California 93106

251. MOLECULAR BEAM STUDIES OF METASTABLE RARE GAS CHEMILUMINESCENT REACTIONS — $52,000 — 01-02
Richard M. Martin
Department of Chemistry

Metastable rare gas chemiluminescent reactions are being studied using a crossed molecular beam optical spectrometer to obtain emission spectra and a crossed molecular beam time-of-flight spectrometer to obtain cross sections as a function of collision energy. The major objectives of this research program are to determine reaction cross sections and product state distributions as a function of collision energy, and to compare these results with theoretical reaction models in order to elucidate the reaction mechanisms. The collisional processes under study include neutral excitation reactions, fluorescent chemiionization reactions, and atom transfer reactions giving excited rare gas halide and oxide molecules. The information to be obtained in this work is of current interest in furthering knowledge of excited state chemistry, and is also of practical importance for understanding the fundamental dynamic processes which occur in excited rare gas reaction systems such as rare gas eximer and excitation transfer lasers.

PRINCETON UNIVERSITY
Princeton, New Jersey 08544

252. DYNAMICAL STUDIES IN MOLECULAR SYSTEMS — $122,631 — 01-02
Herschel Rabitz
Department of Chemistry

The research program has two parts consisting of studies in chemical kinetics and collision dynamics. In the first part on chemical kinetics, the research is concerned with the development and application of sensitivity analysis tools for the understanding of complex chemical mechanisms. Both time and spatially dependent problems are under study with a special emphasis on combustion phenomena. In the latter case, sensitivity techniques are being developed for probing the role of rate constants, transport coefficients, initial conditions and boundary conditions on laboratory observables. The second part of the research in collision dynamics is concerned primarily with the development and application of collision scaling relationships. Scaling can be viewed as a form of inversion which takes laboratory data to a more fundamental underlying level such that it may be used again to produce new predicted observable collision phenomena. A hierarchical approach to collisional scaling is being taken whereby the scaling relations may be employed with various levels of sophistication. Applications to the inversion of collisional relaxation data are being considered.

Chemical Physics, continued

GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, Georgia 30332

253. A KINETIC STUDY OF RADICAL-AROMATIC HYDROCARBON REACTIONS — $60,287 — 01-02
A. R. Ravishankara
Engineering Experiment Station

Improvements in the fundamental understanding of chemical reaction rates and pathways in radical-unsaturated hydrocarbon reaction is the principal objective of this program. Using the technique of (laser/flash) photolysis - (resonance/laser induced) fluorescence, the absolute rate constant measurements for reactions of H, O, OH + aromatic and olefinic hydrocarbon are being carried out as functions of temperature and pressure. By judicious interpretations of observed kinetic isotope effects, the yield and identity of certain products, the temporal profiles of reactant and product concentrations, and the effect of pressure and scavenger concentrations on the rate coefficients, the reaction mechanisms for all the above reactions in the temperature range of 250-1100 K have been elucidated. Furthermore, studies on aromatic free radicals have been initiated. Information gained from these studies is expected to help better utilization of hydrocarbons both as combustibles and as feedstocks for synthetic fuel production, as well as increasing our understanding of hydrocarbon combustion.

WRIGHT STATE UNIVERSITY
Dayton, Ohio 45435

254. THE DIRECT DETERMINATION OF ATOM AND RADICAL CONCENTRATIONS IN THERMAL REACTIONS OF HYDROCARBONS AND OTHER GASES — $55,190 — 01-02
G.B. Skinner
Department of Chemistry

The general goal of this research is to study the kinetics of the atom and free radical reactions that are important in combustion reactions by following the appearance and disappearance of H, O, OH and other such combustion intermediates. H, D and O atoms are currently being measured in shock tube experiments using resonance absorption spectroscopy in the vacuum ultraviolet. Measurements made recently include H and D atom measurements in pyrolysis of dilute mixtures (in argon) of benzene-d_6, toluene-d_8, and mixtures of these compounds with 2,2-dimethylpropane (neopentane). In the experiments with mixtures, H atoms produced by dissociation of neopentane react with the deuterated aromatic compounds. Measurements of H and D concentrations help to clarify the reaction mechanisms. Experiments in which both H and D concentrations are measured in pyrolysis of partially deuterated propene are also being carried out.

RICE UNIVERSITY
Houston, Texas 77251

255. SUPERSONIC METAL CLUSTER BEAMS — $120,000 — 01-02
R. E. Smalley
Department of Chemistry

Laser vaporization of a metal target within a pulsed supersonic nozzle is used in this research to prepare beams of transition metal clusters. This new technique (developed in the previous year of this DOE contract) is perfectly general for even the most refactory metals (eg. tungsten) and readily provides an intense source of bare metal clusters cooled to internal temperatures on the order of 5 K. Current research with this new source centers around the spectral study of small transition metal clusters in order to obtain accurate and definitive measurements of the the metal-metal bond (bond length, dissociation energy, electronic structure, bond angles, vibrational frequencies, etc.). Metal clusters studied thus far include Cr_2, V_2, Ni_2, Cu_2, Cu_3, and Mo_2. The results in the case of Cr_2 and V_2 indicate that the metal-metal bond in this region of the transition series is dominated by strong 3d orbital interaction, resulting in extremely short bond lengths. Nickel and copper, on the other hand, are found to be bound mostly through the 4s orbitals.

Chemical Physics, continued

UNIVERSITY OF CALIFORNIA/SAN DIEGO
La Jolla, California 92093

256. SHOCK-TUBE STUDIES OF IMPORTANT COMBUSTION-REACTION STEPS INVOLVING RADICALS — $60,493 — 01-02
Klaus G. P. Sulzmann
Energy Center

The aim of this research is twofold: (a) the use of shock-tube techniques for the rapid introduction of known intermediate and radical concentrations into a combustion environment in which the individual interactions of these species with other reactants and intermediates can be separated or enhanced for meaningful rate measurements of individual or sub-groups of reaction paths relevant to hydrocarbon combustion, and (b) the use of in situ quantitative spectroscopic measurement techniques for the determination of required species concentration-time histories. As a first step, the only partly understood fate and kinetics of the CH_3-radical is investigated during its donor-pyrolysis and its interactions with O_2 and O-atoms behind reflected shock-waves by using argon-diluted $CH_3CO_2CH_3$, $(CH_3)_2$, CH_3COCH_3 and/or CH_3N_2 as methyl radical donors. Oxidation reactions are initiated by admixing either O_2 or N_2O as an O-atom donor. Quantitative spectroscopic data are obtained by infrared emission (2 channels), by infrared HeXe-laser absorption at 3.508μ, by visible ultraviolet emission (10 channels), and/or by vacuum-ultraviolet absorption.

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

257. VARIATIONAL TRANSITION STATE THEORY — $65,000 — 01-02
Donald G. Truhlar
Department of Chemistry

This research program is an attempt to develop and implement new methods for calculating rate coefficients for chemical reactions from potential energy surfaces. Emphasis is being placed on gas-phase atom-transfer reactions, which are an important reaction type in combustion and atmospheric systems, as well as being of fundamental interest. We are also studying the effect of vibrational excitation of the reactants on chemical reaction rates, and we are studying kinetic isotope effects. A very important aspect of our studies is the inclusion of quantal effects in reaction rate calculations, with special emphasis on tunneling (barrier penetration) and on the dependence of vibrational frequencies on the reaction coordinate. We are developing methods to include tunneling contributions in the limits of small and large reaction-path curvature, as well as a least-action model that is applicable to all cases. Examples of our applications to reactions important in combustion are $OH + H_2 \rightarrow H_2O + H$ and $OH + O \rightarrow H + O_2$.

NATIONAL BUREAU OF STANDARDS
Washington, DC 20234

258. KINETICS DATA BASE FOR COMBUSTION MODELING — $90,000 — 01-02
Wing Tsang and Robert F. Hampson
Chemical Kinetics Division

The aim of this research is to compile, evaluate and publish information on the rate constants for single step chemical processes which are pertinent to the detailed description of hydrocarbon combustion processes. The plan of attack is to start with the simplest molecular systems and then to expand into more complicated situations. All possible reactions are considered. Evaluation involves critical examination of experimental data, comparisons with analogous reactions and expectations from theory. Where data does not exist estimates are made. Results are presented on individual data sheets so as to permit periodic upgrading. Work on methane and ethane oxidation and pyrolysis have now been completed. It should be noted that these reactions form a subset of all combustion processes. Further work will involve continuous updating and expansion into NO_x, CH_3OH and higher hydrocarbon systems.

Chemical Physics, continued

SURFACE ANALYTIC RESEARCH, INC.
Mountain View, California 94043

259. ELECTRONIC STRUCTURE OF HEAVY TRANSITION METAL CARBONYLS — $62,000 — 01-02
Cary Y. Yang

The objective of this research program is twofold. Because of the inherent similarity between transition metal carbonyls and chemisorbed CO on a surface of the same metal, an improved understanding of the carbonyl electronic structure is likely to assist in the study of CO chemisorption. A comprehensive tool for calculating both bound and continuum states of molecules containing heavy elements such as the fifth-row transition metal carbonyls is needed and being developed. The first-year effort consists of ground-state calculations for $W(CO)_6$, $Re_2(CO)_{10}$, $Os_3(CO)_{12}$, and $Ir_4(CO)_{12}$, and the formulation of Dirac-scattered-wave (DSW) continuum states. The metal $d_{3/2}$-$d_{5/2}$ hybridization, which can only be obtained with this fully relativistic SCF-Xα-DSW method, is considerably larger in tungsten, rhenium, and osmium carbonyls than in iridium or platinum ones. All four molecules have similar metal-ligand bonding mechanisms, namely, carbonyl-to-metal donation through 5σ, and back-donation through $2\pi^*$. The continuum states formulation is in progress, with the secular matrix being set up from the boundary conditions.

Atomic Physics

NEW YORK UNIVERSITY
New York, New York 10003

260. ENERGY-RELATED ATOMIC AND MOLECULAR STRUCTURE AND SCATTERING STUDIES — $80,000 — 01-03
Benjamin Bederson
Department of Physics

A program to study atomic and molecular interactions with dc and ac electric fields is in progress, as well as one to study interactions of electrons with highly polar molecules. We have recently completed an extensive study of the electric dipole polarizabilities of selected alkali halide dimers, and are now completing a study of indium ($\sim 12 \times 10^{-24} cm^3$). Similar measurements on thallous halides, additional alkali halides, and some representative very heavy elements, are underway. We also completed our first scattering measurements, using a new scattering apparatus. These involve scattering of slow electrons (~1 to 22 eV) by the highly polar CsBr molecule. Absolute values of "effective" cross sections have been obtained; these can be directly compared with computations by folding the latter into our known "apparatus functions". A systematic study of similar cross sections using molecules possessing a range of dipole moments is also in progress. Extension of ground-state measurements to excited states (for both polarizabilities and molecular scattering) using laser excitation, is now in the preliminary stages of development.

THE UNIVERSITY OF NEW MEXICO
Albuquerque, NM 87131

261. ATOMIC PHYSICS WITH RELATIVISTIC BEAMS — $90,000 — 01-03

Howard C. Bryant
Department of Physics and Astronomy

Exploitation of the relativistic kinematics of an 800 MeV H^- beam at the Clinton P. Anderson Meson Physics Facility (LAMPF) at Los Almos allows the observation, with very little background, of the one and two electron continua and embedded resonant structures. The H^- system is being studied using Doppler-tuned laser probes and motional electric fields, which have so far ranged up to 7 MV/cm, far in excess of those possible using more conventional laboratory techniques. The behavior of the H^- system as a function of both excitation energy and applied field is being carefully mapped out. Energy scale calibration is provided by excitation, with single photon absorption, of the Lyman series in an H^0 beam, derived from the H^- beam by photodetachment. The studies of the ^1P resonant structures in H^- near n=2, the shape and Feshbach resonances, and that of the 2 electron threshold region are proving to be exceptionally challenging to atomic physics theory and more detailed measurements in these regions are planned.

NATIONAL BUREAU OF STANDARDS
Washington, D.C. 20234

262. ELECTRON-ATOM COLLISION STUDIES USING OPTICALLY STATE SELECTED BEAMS — $111,200 — 24 mo. — FY 82-83 — 01-03

Robert J. Celotta and Daniel T. Pierce
Radiation Physics Division

The use of coherence and correlation techniques holds great promise for deepening our understanding of the electron-atom collision process. In particular, the recent rapid advancement in the technologies necessary to produce and detect spin polarization in free electron beams as well as the availability of optical pumping methods which can be used to orient atomic beams make possible electron-atom collision studies where both partners are in optically selected quantum states. This research project will apply such techniques to the electron-alkali system to study: the exchange interaction, the spin orbit interaction, electron correlation in near threshold ionization, resonance effects, inelastic excitation, and super-elastic scattering. A cross-beam apparatus, with both polarized atom (Na) and polarized electron beams, is now in operation. In its first application the spin dependence of the threshold ionization process leading to a sodium ion plus two free electrons in spin selected states is being studied. Subsequent experiments will deal with ionization of the first excited state of sodium and the spin dependence in elastic scattering.

Atomic Physics, continued

COLLEGE OF WILLIAM AND MARY
Williamsburg, Virginia 23185

263. COLLISIONAL DETACHMENT OF NEGATIVE IONS — $75,000 — 01-03
R. L. Champion and L. D. Doverspike
Department of Physics

The fundamental goals of these experimental studies are to determine various cross sections and to develop a general understanding of the collisional dynamics for systems which involve negative ions. The energy range of the experiments is from a few electron volts up to 500 eV. The experiments include measurements of absolute total cross sections, doubly-differential cross sections, and the energy spectra of electrons which are liberated in collisional electron detachment. The processes under investigation include collisional detachment, charge transfer, reactive scattering and inelastic scattering. Emphasis is placed upon developing an understanding of the role of resonances in negative ion-molecule collisions and upon delineating the various collisional processes that may occur in collisions of negative ions with molecular targets. Studies have been completed on the systems $H^-(D^-) + H_2$, D_2, HD and are underway for $H^-(D^-) + CH_2$. The experimental results are coupled with theoretical models to provide a basis for understanding the role of negative ions in various experiments.

UNIVERSITY OF KANSAS
Lawrence, Kansas 66045

264. MANY-BODY PROCESSES IN ATOMIC AND MOLECULAR PHYSICS — $60,000 — 01-03
Shih-I Chu
Department of Chemistry

The fundamental goals of this project are to develop new theoretical formalisms and practical numerical methods for probing intense field atomic and molecular multiphoton processes and predissociation dynamics of van der Waals molecules. A semi-classical many-mode Floquet theory has been developed for nonperturbative treatment of the interaction of a quantum system with several monochromatic oscillating fields. Current work includes; (1) Spectral line shape analysis on the multiphoton absorption spectra of HF and CO molecules, (2) high precision rotational predissociation lifetime determination of Ar-H_2 and Ar-HD van der Waals molecules, (3) development of a complex quasi-vibrational energy and an inhomogeneous differential equation methods for the computation of two-photon dissociation cross sections of vibrationally excited states of H_2^+.

UNIVERSITY OF TOLEDO
Toledo, Ohio 43606

265. SEMIEMPIRICAL STUDIES OF ATOMIC STRUCTURE — $55,000 — 01-03
L. J. Curtis — 24 mo.
Department of Physics and Astronomy — FY 83-84

The structure and properties of very heavy and very highly ionized atoms is being studied through experimental measurements utilizing fast ion beam excitation and through the identification and exploitation of regularities in the data base using precise empirical parametrizations. The use of spectroscopic line intensities to determine thermonuclear plasma temperatures and densities requires laboratory observation and analysis of these systems. The spectroscopic accuracies required are difficult to achieve by purely ab initio theoretical methods for complex many electron systems in this highly relativistic regime. Through the acquisition and systematization of experimental data, regularities and linearities are being utilized to predict a wide variety of atomic structure properties, which are subsequently tested experimentally. During the past year, special emphasis has been given to the prediction of wavelengths and transition probabilities for metastable states in highly ionized atoms that decay by magnetic dipole, electric quadrupole, or spin-mixing processes, which are observed in tokamak spectra.

Atomic Physics, continued

HARVARD-SMITHSONIAN CENTER FOR ASTROPHYSICS
Cambridge, Massachusetts 02138

266. THEORETICAL STUDIES OF HIGHLY IONIZED SPECIES — $95,000 — 01-03
A. Dalgarno

Collisions of multiply-charged ions with neutral gas affect the ionization structure, thermal balance, radiation losses and ion transport in plasmas containing a neutral component. Because the products of the collisions radiate, they can be detected and thereby provide unique diagnostic probes of the environment. We have extended our calculations of the efficiencies of the processes so that their accuracy can be assessed by comparison with experimental data, which are now becoming available. We have made estimates of charge transfer into individual fine-structure states because observations of astrophysical objects show that the separate emission lines can be distinguished readily. We have also explored collisions of positive and negative ions.

UNIVERSITY OF CHICAGO
Chicago, Illinois 60637

267. BASIC STUDIES OF ATOMIC DYNAMICS — $94,000 — 01-03
U. Fano
Department of Physics and
James Franck Institute

This project aims at describing and predicting the correlations and the energy transfers among the variables of atomic and molecular systems. The observed but paradoxical stability of resonant states that are localized on top of potential barriers, rather than on valley bottoms, seems to have been eventually understood. It derives from a general property of light or particle beams focussed about a symmetry axis or plane. Whichever action produces the focussing also confines the associated transverse wave causing it to acquire a discrete stable spectrum. This concept is being applied initially to construct the theory of the quasi-Landau resonances of Rydberg spectra in a magnetic field, but it should bear on all atomic and molecular reactions. Other current research on novel aspects of electron mechanics is progressing regularly.

VANDERBILT UNIVERSITY
Nashville, Tennessee 37235

268. THEORETICAL STUDIES OF ATOMIC TRANSITIONS — $78,000 — 01-03
Charlotte Froese Fischer
Computer Science Department

The present research is part of an ongoing project in atomic structure calculations using the MCHF method. The primary emphasis is on correlation effects. Relativistic effects are estimated using an intermediate coupling calculation based on a Breit-Pauli approximation. The program for computing allowed transition probabilities has been extended to include forbidden transitions of interest in plasma diagnostics. Non-orthogonal orbitals are permitted. An integrated set of programs, capable of executing interactively on minicomputers, has been developed. Several transitions of current interest are being investigated. These include the E2 and M1 transitions between levels of $2p^3$ in the nitrogen isoelectronic sequence. Excellent agreement with the observed fine-structure splitting has been achieved for the $^2D_{5/2} - {}^2D_{3/2}$ and $^2P_{3/2} - {}^2P_{1/2}$ energy separations. Similar calculations for the $3p^3$ levels in the phosphorus sequence are under way. Allowed transitions between doubly excited states of B III are also under investigation. Preliminary studies of changes required to adapt MCHF procedures to photoionization calculations have been made.

Atomic Physics, continued

WAYNE STATE UNIVERSITY
Detroit, Michigan 48202

269. FREE CHARGED PARTICLE BEHAVIOR IN INTENSE LASER FIELDS — $17,000, 18 mo., FY 82-83 — 01-03
David M. Fradkin
Department of Physics and Astronomy

The objective of this project is to perform a theoretical analysis of the effects that intense laser pulses, possible in conjunction with auxiliary electromagnetic field configurations, have on the dynamics of free charged particles. Various models of interaction between particles and fields are being investigated, with particular attention focussed on the amount of momentum-energy transfer to the particle. The effect of radiation reaction, laser polarization, special field configurations, and the nature of asymptotic spin direction change, and magnetic moment behavior are also being investigated. Under special study is the behavior of an otherwise free electron being subjected to two laser fields, propagating in different directions, with different amplitudes and frequencies. A classical treatment of the particle dynamics is being investigated preliminary to a full quantum mechanical treatment. Also under study is the nature of the radiation emitted by such a particle, the intensity of that radiation as a function of the pump laser parameters, its coherence, and also its spectral and angular distribution.

SRI International
Menlo Park, California 94025

270. STUDIES OF AUTOIONIZING STATES RELEVANT TO DIELECTRONIC RECOMBINATION — $72,000 — 01-03
Thomas F. Gallagher
Molecular Physics Laboratory

The goal of this program is the study of doubly excited atomic states of alkaline earth atoms which lie above the lowest ionization limit and thus autoionize. Both the intrinsic properties of the atoms and the effects of external fields are investigated. The approach employed is multistep laser excitaiton of atoms in a thermal beam followed by subsequent detection of the ions and electrons produced by autoionization. The high resolution of the laser affords an excellent spectral probe of the autoionizing levels, and energy analysis of the ejected electrons allows the final state to be unambiguously determined. All theoretical models of dielectronic recombination, the inverse of autoionization, incorporate the above mentioned phenomena, and the data from these experiments should provide the means to make more stringent test of the theory.

UNIVERSITY OF OKLAHOMA
Norman, Oklahoma 73019

271. EXPERIMENTAL AND THEORETICAL STUDY OF VERY LOW INELASTIC PROCESSES IN ELECTRON-MOLECULE COLLISIONS — $86,000 — 01-03
David E. Golden and Michael A. Morrison
Department of Physics and Astronomy

The research program involves a comprehensive theoretical and experimental study of very-low-energy electron-impact excitation of molecules. This research is directed at determining reliable cross sections for molecules of basic scientific interest and of relevance to technological applications such as advanced energy programs. The program seeks to resolve significant discrepancies that exist among the results of various experimental and theoretical investigations of near threshold excitation of molecules by low-energy electrons and to develop a deeper understanding of the physics of this important collision process. In the experimental part of the program absolute differential cross sections for low-energy, electron-impact excitation of these molecules shall be measured using a crossed-beam time-of-flight (TOF) apparatus which is especially suited to low-energy collision studies. The theoretical program entails carrying out accurate ab-initio calculations of cross sections for vibrational and rotational excitation and developing new methodologies for handling collisions with large complex molecular targets in the near-threshold energy regime.

Atomic Physics, continued

UNIVERSITY OF GEORGIA
Athens, Georgia 30605

272. QUANTUM MECHANICAL STUDIES OF HEAVY ION SCATTERING PROCESSES — $48,000 — 01-03
T. G. Heil
Department of Physics and Astronomy

This research program concentrates on low to intermediate energy processes where a quantum mechanical description is most appropriate. Several heavy ion processes involving important constituent reactions that take place in terrestrial and astrophysical plasmas are being studied in detail. Inelastic collisions of protons with many-electron ions are being considered in a quasimolecular formulation. This type of reaction is being considered for use as a probe of proton density and temperature. Charge transfer processes between hydrogen atoms and multiply charged ions by both radiative and nonradiative mechanisms are also being studied. The charge transfer reactions [$C^{2+} + H \rightarrow C^{+} + H^{+} + h\nu$] and [$Al^{3+} + H \rightarrow Al^{2+} + H^{+}$] are being examined in detail.

LOUISIANA STATE UNIVERSITY
Baton Rouge, Louisiana 70803-4001

273. ELECTRON COLLISIONS WITH POSITIVE IONS — $30,000 — 01-03
Ronald J.W. Henry
Department of Physics & Astronomy

The fundamental goals of this project are to delineate the important physical processes which govern electron impact excitation processes for highly stripped impurity ions in high temperature plasmas of interest in thermonuclear reactors. The energy range considered is from the threshold to approximately four times the ionization energy. Calculations are based on a close-coupling expansion which includes the important physical effects of electron exchange and resonances. Calculations are made for inner-shell excitation-autoionization contributions to total ionization for Ti^{+3} and are in good agreement with measurements of Falk et al. Differential electron scattering cross sections for inelastic excitation of Zn^{+} are calculated at energies between 15eV and 100eV. Agreement of theory with the experiment of Chutjian at 75eV is excellent over the measured angular range of 4° to 16°.

ST. JOHN FISHER COLLEGE
Rochester, New York 14618

274. MULTILEVEL RELAXATION PHENOMENA AND POPULATION TRAPPINGS — $109,000 24 mo. FY 82-83 — 01-03
F. T. Hioe
Department of Physics

This research program is directed toward the studies of preparing multilevel atoms in high-lying levels using one or more laser pulses, and of multiphoton relaxation processes. The main results this year have been the discovery of unexpected population inversion procedures which give a generalized interpretation of adiabatic following, and the analytic formulation of specific pulse sequences incorporating both amplitude and phase modulation which give specific degrees of inversion of multilevel atoms. The precise analytic nature of these results opens the ways for a comprehensive study of multilevel photon-echo effects which are important for understanding multilevel relaxation processes.

Atomic Physics, continued

THE UNIVERSITY OF TEXAS AT AUSTIN
Austin, Texas 78712

275. KINETIC STUDIES FOLLOWING STATE SELECTIVE LASER EXCITATION — $68,000 — 01-03
John W. Keto
Department of Physics

Electronic energy transfer from xenon atoms and excimers is studied following selective excitation by multiphoton laser excitation. Reactions at higher pressures where termolecular processes are observed are being emphasized. Initial experiments are studying radiative lifetimes and quenching of $5p^56p$ xenon atoms in collisions with xenon and other rare gases. Accurate potential curves for xenon excimers are obtained by comparison of two-photon spectra with line broadening theories. Comparisons are made over a broad range of temperature and pressures. Collisional deactivation rates are being measured. These rates are found to be dependent upon laser frequency. Atoms which absorb in the red wing of an absorption are excited as collision pairs at a unique inter-nuclear separation; hence the laser prepares the reactant selectively on the collision surface. Experiments studying laser controlled reactive transfer are planned.

SMITHSONIAN ASTROPHYSICAL OBSERVATORY
Cambridge, Massachusetts 02138

276. MEASUREMENTS OF IONIZATION BALANCE PARAMETERS IN ATOMIC IONS — $94,000 — 01-03
John L. Kohl
Atomic and Molecular Physics Division

The purpose of this research program is to measure the basic atomic parameters that govern the charge distribution of atomic ions in high temperature plasmas. The present research efforts are directed toward measurements of absolute cross sections for dielectronic recombination of a multiply charged atomic ion and a free electron. This process is believed to dominate the ionization balance of impurity ions in potential controlled thermonuclear plasmas. The measurements utilize inclined electron and ion beams and, in the experiments, ion-photon pairs of recombined ions and stabilizing photons from individual dielectronic recombination events are measured in coincidence to ensure the correct identification of the detected process. The immediate goal is to measure the dielectronic recombination cross section for C^{4+}. A new experimental arrangement is fully operational and the actual measurements of dielectronic recombination are underway.

CORNELL UNIVERSITY
Ithaca, New York 14853

277. EXPERIMENTAL STUDY OF INTERACTIONS OF HIGHLY CHARGED IONS WITH ATOMS AT keV ENERGIES — $190,000 — 01-03
Vaclav O. Kostroun
Nuclear Science and Engineering Program

The objective of this program is to investigate interactions of highly charged ions with atoms at keV collision energies ($v/c<e^2/\hbar c$). Low energy multiply charged ion beams are generated by an electron beam ion source (EBIS), by successive electron impact ionization of ions trapped in an intense, magnetically confined electron beam. Thus far, $\sim 10^8$ particle/pulse beams of 250 to 800 qeV C^{+5}, N^{+6} and O^{+6} have been produced by a 2.5 kV, 275 mA electron beam in an EBIS designed and constructed in this laboratory. Charge transfer collisions between multiply charged C, N and O ions and helium and molecular hydrogen and deuterium are being investigated by energy gain spectroscopy. The energy spread of a 650 qeV C^{4+} beam after a 0.5 mm slit 30 cm downstream of a 15 cm radius 60° analyzing magnet is $\sim$ 1 eV. The charge and energy selected beam passes through a gas jet interaction region and the emergent beam is analyzed by an electrostatic 127° charged particle analyzer. Measurements of electron capture cross sections into specific quantum states of the projectile as a function of its kinetic energy are in progress. In addition to these studies, preliminary design of a larger superconducting solenoid EBIS initially capable of producing Ar^{18+} has been carried out.

Atomic Physics, continued

UNIVERSITY OF MISSOURI-ST. LOUIS
St. Louis, Missouri 63121

278. LOW ENERGY ION-NEUTRAL COLLISIONS — $65,000 — 01-03
J. J. Leventhal
Department of Physics

This experimental program is designed to investigate energy transfer and energy conversion in atomic and molecular interactions. Current emphasis is on interactions involving atoms in specific excited electronic states which are produced by laser photoexcitation. By using both spectral analysis of the radiation emitted by the reaction products and mass analysis of ionic products nearly complete characterization of the interactions can often be achieved. Of particular interest at this time is the examination of processes that are steps in the complicated sequence of microscopic reactions that collectively produce macroscopic effects, such as plasma formation, by coupling laser energy to gases or vapors.

UNIVERSITY OF ARKANSAS
Fayetteville, Arkansas 72701

279. A THEORETICAL STUDY OF ELECTRON CAPTURE IN ION-ATOM COLLISIONS — $40,000 — 01-03
17 mo.
FY 82-83
M. Lieber and F. T. Chan
Department of Physics

Electron capture processes in ion-atom and ion-ion collisions, e.g. $A^+ + B \rightarrow A + B^+$, are of importance to areas of research, such as the controlled fusion energy program, astrophysics, and atmospheric phenomena. As a prototype of a rearrangement collision which is experimentally accessible, charge exchange has been studied since the earliest days of quantum mechanics, but the difficulty of calculation has limited theoretical progress. Recent work has shown that eikonal techniques can be successfully applied to problems of this type, and have surprising power and simplicity. Calculations are being performed on: (A) Simultaneous capture of two electrons in He^{++} collisions with neutral atoms; (B) The connection between the eikonal approximation and asymptotic behavior of the wave function; (C) The effect of stark-mixing of energy levels on electron capture cross sections for capture into a subshell.

KANSAS STATE UNIVERSITY
Manhattan, Kansas 66506

280. ATOMIC PHYSICS OF STRONGLY CORRELATED SYSTEMS — $70,933 — 01-03
Chii-Dong Lin
Department of Physics

This program is directed toward the understanding of correlations of two-electron atoms in hyperspherical coordinates and the development of practical codes for computing inelastic cross sections in ion-atom collisions. The Stark shift and Stark quenching of two-electron resonances in a strong external electric field are being investigated. A complete classification scheme for doubly excited states is being developed. The modified atomic-orbital model (AO+) is generalized to include excitation, charge transfer and ionization processes for calculating inelastic ion-atom collisions at intermediate and low velocities.

Atomic Physics, continued

UNIVERSITY OF NEBRASKA/LINCOLN
Lincoln, Nebraska 68588-0111

281. HYPERSPHERICAL COORDINATE THEORY OF TWO-ELECTRON ATOMIC PROCESSES — $60,000 — 01-03
Joseph Macek and Anthony F. Starace
Department of Physics and Astronomy

A new hyperspherical coordinate framework for treating two electron atomic processes is proposed. The Fock expansion for a two electron wavefunction near R = 0 is matched at a finite radius R_0 to a linear combination of separable hyperspherical channel wavefunctions. This procedure is proposed to solve the problem introduced by the too repulsive effective potentials in most previous hyperspherical treatments and thus to put the hyperspherical coordinate method on a fully quantitative basis. The Fock coefficients have been obtained numerically and will be used to calculate photoabsorption by He and H^- as well as elastic electron scattering by H.

MOREHOUSE COLLEGE
Atlanta, Georgia 30314

282. THEORETICAL INVESTIGATION OF ELECTRON-ION INTERACTION — $43,836 — 01-03
Alfred Z. Msezane
Department of Physics

The purpose of this investigation is to identify and calculate dominant physical mechanisms underlying the processes of electron impact excitation and ionization of ions using the close-coupling approximation. Both total and differential cross sections are calculated and compared with measurements. In particular, detailed numerical studies are carried out to investigate the extent of contribution of the physical processes of inner-shell excitation-autoionization, and inner-shell resonant-excitation-double autoionization to the total ionization cross section of Ti^{+3} important in CTR plasmas. An accurate configuration - interaction wave function of the target is used, a wave function which is constructed to give the same values for the oscillator strengths in the length and velocity formulations.

NATIONAL BUREAU OF STANDARDS
Boulder, Colorado 80303

283. ATOMIC AND MOLECULAR COLLISION PROCESSES — $93,000 — 01-03
David W. Norcross
Quantum Physics Division - 525

The focus of this program is the physics of low-energy collisions of electrons with atom, ions, and molecules, with an emphasis on detailed computational studies. High precision calculations for elastic scattering by neutral helium are being extended to near-threshold excitation. Core polarization effects as the cause of the serious discrepancy between theory and experiment for excitation of Be^+ are being investigated. The effects of zero-point averaging and polarization in vibrationally elastic scattering by HF have been shown to be small. A new parameter-free correlation-polarization model for molecular scattering based on free-electron-gas theory is being tested for several molecules, including H_2, N_2, and HCl. Calculations of vibrational excitation of HCl are in progress.

Atomic Physics, continued

UNIVERSITY OF TENNESSEE/KNOXVILLE
Knoxville, Tennessee 37996

284. PRODUCTION AND DESTRUCTION OF METASTABLE NEGATIVE IONS — $42,000 — 01-03
David J. Pegg
Department of Physics

This research program is designed to investigate the production and destruction of metastable negative atomic ions. In particular we begin our measurements on Ca^- where the $4s4p^2\ ^4P$ state is theortically predicted to be bound and metastable against allowed radiative and autodetachment decay mechanisms. Our source of negative ions is a fast moving beam and we plan to use electron spectroscopic techniques to study the energy of electrons detached in flight by the processes of autodetachment, collisional detachment and photodetachment.

JACKSON STATE UNIVERSITY
Jackson, MS 39217

285. SPECTROSCOPY OF TRAPPED MOLECULAR IONS — $50,000 — 01-03
J. Perkins, G. Miller
Chemistry Department

The goal of this project is to provide spectroscopic data that will help document those characteristics of molecular ions responsible for the large cross sections accompanying ion-molecule reactions. Using laser induced fluorescence (LIF), energy level and lifetime measurements are made of various small molecular ions, e.g., O_2^+, CO^+, CH^+ and CH_3^+. The ions are prepared by fragmentation of parent neutral gases through electron impact using a Pierce-type pulsed electron gun. The ions are mass selected by and trapped in a quadrapole ion trap long enough to carry out the spectroscopic measurements. Attempts are made to study intra- and intermolecular energy exchange involving electronic, vibrational and rotational motions of these ions. Light intensity measurements are made using a dye laser and the results are used to determine excited state lifetimes in the order of tens of milliseconds.

UNIVERSITY OF ROCHESTER
Rochester, New York 14627

286. NONLINEAR OPTICS WITH BROAD-BAND LASERS — $59,831 — 01-03
Michael G. Raymer
The Institute of Optics

Experiments are being carried out to understand the statistical properties of broad-band laser radiation, and the effects of using such radiation in several areas of nonlinear optics. Intensity fluctuations and mode correlations are being studied in both cw and pulsed broad-band dye lasers via intensity autocorrelation and spectral measurements. Such broad-band lasers are used to pump stimulated Raman amplification and coherent anti-Stokes Raman scattering in hydrogen gas. Intensity and field cross-correlations which develop between pump and probe laser beams in these processes are being observed using an intensity cross-correlator and a nonlinear interferometer based on the interference of beams produced at the sum-frequency of the two beams of interest.

Atomic Physics, continued

KANSAS STATE UNIVERSITY
Manhattan, Kansas 66506

287. ATOMIC PHYSICS WITH HIGHLY CHARGED IONS — $490,000 — 01-03
Patrick Richard
James R. Macdonald Laboratory
Department of Physics

High velocity, highly charged ions produced by the 6 MV KSU tandem Van de Graaff are used to study charge transfer, ionization and excitation in ion-atom collisions. During this contract period the impact parameter dependence of delta electrons, recoil ions, and Auger electrons have been studied for nearly symmetric F^{q+} - Ne collisions. The final state populations in single- and double-electron transfer have also been studied. Resonant transfer excitation is being studied by a high resolution x-ray spectroscopy method. The high velocity beams have been used to measure the 2s Lamb shift and the 1s Lamb shift in one-electron ions. The so-called "Thomas peak" in the angular distribution of the scattered ion in electron capture predicted by a second Born calculation has been observed for the first time in H^+ + He collisions. Energy gain spectroscopy and capture cross sections, using low velocity highly charged ions produced by the recoil ion method, have been studied for several systems with some emphasis on atomic hydrogen and Li targets.

UNIVERSITY OF NORTH CAROLINA
Chapel Hill, North Carolina 27514

288. EXPERIMENTAL STUDIES OF ATOMIC INNER SHELL IONIZATION PHENOMENA — $63,000 — 01-03
S. M. Shafroth
Department of Physics and Astronomy

This program is designed to study inner-shell vacancy production in ion-atom collisions, and subsequent decay via x rays or Auger electrons. Primary emphasis is on experiments relating to dielectronic recombination. Fast highly stripped ions are produced by the TUNL FN tandem Van de Graff and sputter ion source. Thus conditions in magnetic confinement fusion devices are simulated, except that the electrons corresponding to plasma electrons are bound in gas atoms and have relatively little kinetic energy whereas the fast ions have the same velocity as the plasma electrons which give rise to dielectric recombination. This process has been called Resonant Transfer and Excitation (RTE). Cross sections for RTE are being measured for a variety of collision systems by means of the x ray-charge changed beam coincidence method. A set of four parallel plate avalanche detectors has been constructed so that projectiles which have gained or lost one or two electrons can be measured in coincidence with projectile K x rays and radiative electron capture (REC) identified by radiation of a continuum type. REC gives a signature for nonresonant excitation of K electrons and electron capture (NTE). Extensive calculations for RTE and NTE are underway.

UNIVERSITY OF COLORADO
Boulder, Colorado 80309

289. NEAR-RESONANT ABSORPTION BY ATOMS IN INTENSE FLUCTUATING FIELDS — $68,659 — 01-03
Stephen J. Smith
Joint Institute for Laboratory Astrophysics

This research is directed to the measurement of photon absorption by atoms immersed in very intense laser radiation fields, near an atomic resonance. A primary objective is the accurate comparison of atomic absorption in a strong monochromatic field with the absorption in a strong field on which statistically well-characterized frequency fluctuations are superimposed. A hybrid system of electro-optic and acousto-optic modulators is used to impose laser bandwidths up to 30 MHz, and bandshapes out to 1 GHz from line center, on a single-mode laser beam. Lineshapes ranging from Gaussian to Lorentzian are synthesized by controlling the time scale of the fluctuations. The role of fluctuations in nonlinear atomic absorption is measured in the two-photon 3^2S-4^2D transition in sodium, in a Doppler-free configuration: and also in the saturated $3S_{1/2}(F=2,M_F=2) \rightarrow 3P_{3/2}(F=3,M_F=3)$ transition in a highly collimated atomic beam using an optical double resonance technique to study broadening, shifting and splitting of the upper level as a function of laser intensity, detuning, and fluctuation parameters (linewidth and lineshape).

Atomic Physics, continued

RICE UNIVERSITY
Houston, Texas 77251

290. ATOMIC AND MOLECULAR SCIENCES — $175,000 — 01-03
G. K. Walters and N. F. Lane
Department of Physics

This program emphasizes studies of structure and interactions of excited atoms, molecules, electrons and ions. Research areas include reactions and radiative lifetimes in atomic and molecular systems of high-efficiency laser promise, spin dependence in electron-atom scattering and understanding of spectra and collisonal effects of interest in plasma physics and controlled thermonuclear reaction technology. Specifically, time resolved spectroscopy of alkali-halide excimers excited by synchrotron radiation yields stimulated emission cross-sections, formation and quenching rates for excimer laser transitions. Experiments in a flowing afterglow apparatus are directed toward studies of Penning and photoionization of alkali atoms and small clusters, electron exchange in polarized electron-atom/molecule collisions, and new approaches to electron spin polarimetry. Recent theoretical results include cross sections for: radiative charge-transfer collisions between He^{++} ions and H atoms; inelastic electron-ion and ion-ion collisions in a dense, hot plasma; energy transfer in collisions of highly excited atoms with molecules; and Penning ionization of sodium atoms by metastable helium collisions.

TEXAS A&M UNIVERSITY
College Station, Texas 77843

291. X-RAY EMISSION IN HEAVY-ION COLLISIONS — $65,000 — 01-03
R. L. Watson
Cyclotron Institute and
Department of Chemistry

High resolution x-ray spectral measurements are being performed for the purpose of investigating (a) rapid electron transfer in light elements following multiple ionization by fast heavy-ion impact, (b) excitation and x-ray emission from np states of fast heavy ions in gaseous and solid media, and (c) alignment of P states in ion-atom collisions. Spectra are obtained using a variety of beams ranging from protons to argon ions provided by the Texas A&M variable energy cyclotron. The objectives of these experiments are to obtain a basic understanding of the processes responsible for chemical effects on x-ray satellite and hypersatellite structure, and to characterize solid state influences on x-ray emission from few-electron heavy ions, including alignment and possible coherence effects.

Chemical Energy

YALE UNIVERSITY
New Haven, Connecticut 06511

292. STUDIES OF THE HYDROGENATION OF SMALL UNSATURATED MOLECULES USING ORGANO-METALLIC CLUSTER COMPOUNDS AS CATALYSTS — $78,000 — 02-01
Richard D. Adams
Department of Chemistry

This research project is focused on the mechanisms of activation and hydrogenation of small heteronuclear unsaturated molecules like CO and CO_2 by polynuclear transition metal complexes. Special emphasis is being placed on the importance of multinuclear bridging coordination forms in ligand activation. The products of selected reaction sequences are being investigated by IR and NMR spectroscopies and are being structually characterized by single-crystal x-ray diffraction analyses.

UNIVERSITY OF NORTH CAROLINA/CHAPEL HILL
Chapel Hill, North Carolina 27514

293. HEATS OF FORMATION OF GAS PHASE ORGANO-SULFUR MOLECULES AND IONS MEASURED BY PEPICO — $67,670 — 02-01
Tomas Baer and Slayton A. Evans, Jr.
Department of Chemistry

The goal of this research program is to determine accurate heats of formation and structures of organosulfur molecules and ions. The results obtained are of fundamental chemical interest, as well as of importance in the removal of sulfur containing molecules from coal. Some of the species being investigated include HCS^+, H_2CS^+, CH_2SS^+, and CH_3CHS^+. Heats of formation are obtained from fragment ion onsets in photoionization scans. In favorable circumstances, some structural information can be obtained from ion lifetime measurements obtained from Photoelectron photoion coincidence (PEPICO). However the more accurate structures are determined by ab initio calculations. These results are related to the fundamental bonding interactions between S-S and O-O bonds which are being investigated by ^{17}O and ^{33}S NMR. The latter technique is also being developed into a rapid analytical method for determining the form of oxidized sulfur in organic mixtures.

Brigham Young University
Provo, Utah 84602

294. METAL SUPPORT INTERACTIONS: THEIR EFFECTS ON CATALYTIC PROPERTIES OF COBALT — $48,689 9 mo. — 02-01
Calvin H. Bartholomew
Department of Chemical Engineering

Metal-support interactions and their effects upon adsorption and activity/selectivity properties of cobalt are being investigated. The objectives of this research are to (i) determine the effects of cobalt-support interactions on dispersion, oxidation state and adsorption properties of cobalt; (ii) correlate the catalytic properties for hydrocarbon synthesis on cobalt with dispersion, oxidation state and behavior of adsorption of CO and H_2 and (iii) measure directly the extent of interaction of various supports with iron and cobalt using Moessbauer Spectroscopy. The proposed work features a comprehensive, quantitative experimental investigation of Co on Al_2O_3, SiO_2, TiO_2, MgO, and carbon supports with careful characterization of the physical and chemical, bulk and surface properties of each catalysts with BET, H_2 and CO chemisorption, XRD, TEM, TPD, and TPR measurements. Recent results provide evidence that dispersion and support significantly influence adsorption and CO hydrogenation activity/selectivity properties of cobalt.

Chemical Energy, continued

PURDUE UNIVERSITY
W. Lafayette, Indiana 47907

295. REDUCTION OF AROMATIC COMPOUNDS DERIVED FROM COAL BY CALCIUM — $55,000 — 02-01
Robert A. Benkeser
Department of Chemistry

A new reducing system consisting of calcium dissolved in a mixture of methylamine-ethylenediamine has been developed for the reduction of aromatic compounds that can be derived from coal. Hydrocarbons like tetralin, *m*- and *p*-xylene and indane are reduced in excellent yields by the calcium system to a crude product containing 88% or better of a single alkene. Optimal experimental conditions have been developed for the reduction of anthracene to 1,2,3,4,5,6,7,8,9,10-decahydroanthracene, tetralin to $\Delta^{9,10}$ octalin, *p*-xylene to 1,4-dimethylcyclohexene and indane to 4,5,6,7-tetrahydroindane. Surprisingly, durene is reduced by the calcium reagent to 1,2,4,5-tetramethyl-1,4-cyclohexadiene in excellent yield. The syntheses developed for the five aforementioned cyclic alkenes represent the best methods presently available for preparing these compounds. The calcium procedure fails almost entirely to reduce internal alkenes to alkanes. Internal alkynes, however, like 2-nonyne and 4-octyne are reduced quite cleanly to the corresponding *trans*-alkenes. The function of the dual solvent system is under active investigation.

UNIVERSITY OF PITTSBURGH
Pittsburgh, Pennsylvania 15261

296. THE CARBIDIC AD-LAYER AS RATE CONTROLLING FACTOR IN CO/H_2 CATALYSIS — $154,000 — 24 mo. — FY 83-84 — 02-01
Paul Biloen
Department of Chemical/Petroleum Engineering

The objective of this program is to assess the reactivity and abundance of reaction intermediates present at the surface of CO/H_2 converting catalysts during steady-state catalysis. The central question which is being addressed is to what extent carbonaceous side products control the abundancy of reaction intermediates. In a typical experiment the isotopic constitution of the feed is being changed abruptly (e.g., $^{12}CO/H_2 \rightarrow {}^{13}CO/H_2$). This leads to a transient phenomenon: the displacement of ^{12}C by ^{13}C, first in the catalyst ad-layer and then in the product. The rates of displacement contain transient-kinetic information regarding the abundancy and reactivity (i.e., lifetime) of reaction intermediates. With ^{12}CO and ^{13}CO exhibiting essentially identical reactivity, the steady-state of the system is essentially not affected by the isotopic switch. In the present setup, the rate of isotopic substitution in product is being monitored by on-line mass spectrometry. Under construction is a setup to combine this with an in-situ IR monitored rate of isotopic substitution in the reactive ad-layer.

STANFORD UNIVERSITY
Stanford, California 94305

297. CATALYZED GASIFICATION OF CARBON — $152,407 — 24 mo. — FY 82-83 — 02-01
Michel Boudart
Department of Chemical Engineering

The palladium catalyzed conversion of amorphous carbon to a graphitic form has been studied in vacuo and in situ by transmission electron microscope and electron diffraction. Throughout the process, the metal particles appear fluidlike but remain crystalline. There now appears a common thread through a number of phenomena involving a catalyst-carbon interface (CCI): the catalytic gasification of carbon, as reported by us last year, where carbon-carbon bonds are broken at the CCI; the formation of filamentous carbon where carbon-carbon bonds are formed at the CCI; and in the catalytic conversion of amorphous to graphitic carbon where carbon-carbon bonds are both broken and later re-made at different locations of the CCI. The link between those phenomena is the acceleration by the catalyst of the breaking or making of carbon-carbon bonds in the presence or in the absence of reactive gases adsorbed on the carbon or the metal.

Chemical Energy, continued

WAYNE STATE UNIVERSITY
Detroit, Michigan 48202

298. SYNTHESIS, STATIC, AND REACTIVE CHARACTERIZATION OF SUPPORTED ORGANOMETALLICS — Total $84,000 — 02-01

Alan Brenner
Department of Chemistry

Previous research dealing with the synthesis and reactivity of supported carbonyl complexes is being greatly expanded. During the past year glass reaction systems have been replaced with state of the art metal systems combining high purity and the ability to operate between 10^{-7} torr and 1000 psi. Studies of Fischer-Tropsch synthesis at typically 350 psi over catalysts derived from supported $W(CO)_6$ show activities 100-fold higher than for traditional (reduced salt) catalysts of W. Both Mo and W carbonyls also show large enhancements in activity for the hydrogenation of benzene compared to their traditional analogs. H_2-D_2 exchange over alumina and supported $Mo(CO)_6$ has been studied. Contrary to published data, reaction on alumina involves surface hydroxyl groups and the rate of exchange becomes very low if the alumina is activated above 1000 °C. $Mo(CO)_6$ activated to form $Mo(CO)_3$ is of low activity for exchange, but further decomposition results in very high activity. Photolytic activation of $Mo(CO)_6$ has also been studied as an alternative to thermal activation as a route to atomically dispersed metal. However, after facile removal of three ligands the rate of photolysis drops to a very low value.

NORTHWESTERN UNIVERSITY
Evanston, Illinois 60201

299. SUPPORTED f-ELEMENT ORGANOMETALLIC COMPLEXES: SURFACE CHEMISTRY AND CATALYSIS — $125,000 — 02-01

Robert L. Burwell, Jr., Tobin J. Marks — 24 mo.
Department of Chemistry — FY 82-83

This project represents a study of the surface chemistry and catalytic activity of organoactinide complexes deposited on oxide supports. Two complexes, M = Th,U in $M[(CH_3)_5C_5]_2(CH_3)_2$ had been found to give very fast hydrogenation of propylene at -63°C and polymerization of ethylene at 25°C. $Th[(CH_3)_5C_5]_2H_2$ dimer has now been found to exhibit similar activity for hydrogenation, but $U[(CH_3)_5C_5]_2(CH_3)Cl$ has only 5% as much activity. Poisoning experiments with CO indicate that only a few percent of the U or Th atoms become active sites for the above reactions. During activation, a small fraction of $U[(CH_3)_5C_5]_2(CH_3)_2$ loses methane to form $U{=}CH_2$ probably stabilized by interaction with surface Al-O. It is not a good catalyst for olefin metathesis.

NORTHWESTERN UNIVERSITY
Evanston, Illinois 60201

300. THE PROPERTIES OF SUPPORTED METAL CATALYSTS — $65,000 — 02-01

John B. Butt, Robert L. Burwell, Jr.
and Jerome B. Cohen
Ipatieff Laboratory

This research program is aimed at enlarging our understanding of the physical and catalytic characteristics of supported metal catalysts consisting of highly dispersed (1-10 nm) particles of metal on a high area, porous oxide support. During the past year study of the hydrogenation of propylene as influenced by the nature of the pretreatment of Pt/SiO_2 and Pd/SiO_2 catalysts was completed. The preparation of Co, Rh and Co-Rh mixed elements on SiO_2 by decomposition of carbonyls was completed and the hydrogenolysis of methylcyclopropane on the Rh/SiO_2 was investigated. A combined synchrotron-x-ray diffraction EXAFS study was completed on Pt/SiO_2 and Pd/SiO_2, with special attention given to interactions with O_2. A new high-low temperature x-ray chamber was completed that allows in situ studies from -100 to +500 °C under reaction or pretreatment conditions. Current characterization is being carried out on the Co, Rh and Co-Rh systems.

Chemical Energy, continued

UNIVERSITY OF WISCONSIN, MADISON
Madison, Wisconsin 53706

301. MECHANISTIC STUDIES RELATED TO THE METAL CATALYZED HYDROGENATION OF CARBON MONOXIDE TO HYDROCARBONS
Charles P. Casey
Department of Chemistry

$170,000
24 mo.
FY 82-83

02-01

The synthesis of organometallic compounds which contain functional groups similar to those proposed in homogeneous and heterogeneous catalyzed carbon monoxide reduction is being carried out so that the properties and reactions of these species can be studied. This basic information should contribute to the understanding and eventual design of catalysts for the reduction of carbon monoxide. Detailed studies of the synthesis and reactions of metal formyl compounds (M-CO-H) and hydroxymethyl metal compounds (MCH_2OH) [models for intermediates in the homogeneous hydrogenation of CO] are being carried out. Compounds with CH_3, CH_2, and CH groups bridging between two iron atoms have been synthesized as models for intermediate in the heterogeneous catalysis of CO hydrogenation. Carbon-carbon bond forming reactions of the CH compounds with alkenes and with CO are being explored. Several heterobimetallic compounds linked by a heterodifunctional ligand have been synthesized. Their reaction with hydrogen is being studied as a possible route to heterobimetallic dihydrides that might serve as catalysts for CO reduction.

INDIANA UNIVERSITY
Bloomington, Indiana 47405

302. METAL ALKOXIDES - MODELS FOR METAL OXIDES
Malcolm H. Chisholm
Department of Chemistry

$146,500
24 mo.
FY 83-84

02-01

Structural analogies between polynuclear metal alkoxides and metal oxides have been noted, with the former providing models for subunits within the extended networks of the latter. An extensive organometallic chemistry supported by alkoxy ligands is emerging. Their facile interconversion between terminal and bridging positions and between σ^2 and ($\sigma^2 + \pi^2$) donors allows for easy uptake and release of substrate molecules. Key findings during the 1982/83 period are: (i) the cleavage of C≡O to carbido and oxo tungsten alkoxide clusters; (ii) the coupling, co-coupling and sometimes metathesis-like reactions (M ≡ W) between C≡C, C≡N and M≡M bonds in $M_2(OR)_6$ compounds; (iii) unusual β-hydrogen effects in dinuclear alkyl-alkoxides of molybdenum and (iv) the isolation of Mo-Mo quadruply bonded compounds supported by alkoxide ligands.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, New York 12181

303. HOMOGENEOUS CARBON MONOXIDE FIXATION
Alan R. Cutler
Department of Chemistry

$185,000
24 mo.
FY 83-84

02-01

Organometallic complexes containing C_1 alkoxycarbonyl and C_2 carboalkoxymethyl ligands derived from terminally bound CO are being synthesized in order to delineate those coordinated ligand reactions and their intermediates that are viable for CO hydrogenation. The metalloester $FpCO_2CH_3$, derived from $FpCO^+$ or from Fp_2Mg/CO_2, serves as the common template in converting either CO or CO_2 into the C_1 alkyl ligand on $FpCH_2OCH_3$; Fp = $(\eta\text{-}C_5H_5)Fe(CO)_2$. The activated ester $FpC(OCH_3)_2^+$ thus adds hydride and gives its stable formylacetal $FpCH(OCH_3)_2$, which subsequently affords the desired $FpCH_2OCH_3$. The methylidene salt $FpCH_2^+$ (generated from $FpCH_2OCH_3$) picks up exogeneous CO, ascertained by a ^{13}C labeling study, and gives the stable (η^2-C,C) ketene complex $Fp(CH_2CO)^+PF_6^-$; this complex abstracts methoxide from methanol (or even $FpCH_2OMe$) and provides the carbomethoxy methyl $FpCH_2CO_2CH_3$. This ketene complex, which effectively derives from two carbonyls, therefore serves as an efficient source of a C_2 alkyl ligand that is important in CO fixation studies.

Chemical Energy, continued

UNIVERSITY OF COLORADO
Boulder, Colorado 80309

304. STUDIES OF NEW ELIMINATION REACTIONS OF METAL COMPLEXES — $89,657, 24 mo., FY 82-83 — 02-01
Mary Rakowski DuBois
Department of Chemistry

This project is investigating elimination and rearrangement reactions of alkyl substituents on μ_2-sulfido ligands in dimers of the general types $[CpMoSSR]_2^n$ and $[CpMo(SR)_2]_2^n$ (n=0,-1,-2). It has been proposed that the sulfido ligands and metal ions may participate in these reactions to provide low energy pathways for new reaction types. The complex $[(CpMo)_2(S_2CH_2)(\mu\text{-}S)(\mu\text{-}SCH_3)]^-$, I, has been synthesized, and each of its two one-e$^-$ reduction products has been characterized. Protonation of $[I]^{-2}$ produces $(CpMo)_2(S_2CH_2)(\mu\text{-}SH)(\mu\text{-}SCH_3)$, II, which reacts with protons to form hydrogen and I. II also reacts under N_2 at 70°C to eliminate methane. Certain alkenyl substituents undergo unusual rearrangement reactions under nitrogen at 25°C in $CDCl_3$. For example, the 1,2 butene dithiolate ligand in $(CpMo)_2(\mu\text{-}S_2CH_2)(SCH{=}C(C_2H_5)S)$ isomerizes to form a coordinated 2-butene-3,4-dithiolate ligand. When the system is placed under hydrogen, cis 2-butene is produced exclusively, and under deuterium, deuterated (d_2-d_8) cis 2-butenes are formed. The relevance of these reactions to those catalyzed by metal sulfide surfaces is being investigated.

UNIVERSITY OF TEXAS/AUSTIN
Austin, Texas 78712

305. STUDY OF FISCHER-TROPSCH SYNTHESIS THROUGH THE USE OF SURFACE INTERMEDIATE SCAVENGERS — $54,965 — 02-01
John G. Ekerdt
Department of Chemical Engineering

The goals of this program are to identify reaction intermediates involved in synthesis gas conversion and to elucidate the reaction mechanisms. Pyridine is used to scavenge alkyl fragments from a silica supported iron catalyst during Fischer-Tropsch synthesis. The distribution of scavenged fragments establishes that alkyl fragments are the reaction intermediates involved in chain growth and are the immediate precursors to hydrocarbon products. Amines are being used in attempts to scavenge acyl species which may be present and may be involved in alcohol formation and/or chain growth. Direct CO hydrogenation into branched alkanes, isosynthesis, is being investigated over zirconia. Differential reactor studies establish the kinetics and primary products. These experiments suggest that normal and iso C_4 olefins form in a stepwise manner from a common intermediate. Temperature programmed studies of the interaction of synthesis gas with ZrO_2 suggest that CO reacts with surface hydroxyl groups to form formate and methoxide species at one atmosphere. The importance of these C_1 species in C_4 formation is being investigated.

COLORADO STATE UNIVERSITY
Fort Collins, Colorado 80523

306. CHEMICALLY MODIFIED CARBON, PLATINUM, AND NICKEL ELECTRODES — $60,000 — 02-01
C. Michael Elliott
Department of Chemistry

New chemically modified electrodes and related solution chemistry are under study in this research. The goals are to alter the kinetics of electrode reations in a useful way. Of primary interest is the catalysis of various kinetically inert small molecules that are of economic interest; in particular, the respective four electron and six electron reductions of dioxygen and dinitrogen. Different synthetic procedures appropriate for each of the materials under study are being investigated in order to chemically bind the potential catalyst to the surfaces of bulk electrode materials. Our primary emphasis is the development of polymer coated electrodes containing the potential catalyst and/or other electroactive materials. Several such electrodes have been prepared and are under active investigation. A number of novel metalloporphyrin compounds have been prepared and their catalytic activity is presently under investigation both in solution and polymer bound. The primary methods of investigation of these surfaces are electrochemical, including such techniques as chronoamperometry, cyclic voltammetry and the rotated disk electrode technique.

Chemical Energy, continued

UNIVERSITY OF CALIFORNIA, IRVINE.
Irvine, California 92717

307. SYNTHESIS, CHEMISTRY AND CATALYTIC ACTIVITY OF LANTHANIDE METALS IN UNUSUAL OXIDATION STATES AND COORDINATION ENVIRONMENTS — $66,000 — 02-01
William J. Evans
Department of Chemistry

The objective of this research is to identify the special chemical properties of the lanthanide metals (14 heavy metals which are mined in California) and to exploit this unique chemistry to develop (a) new materials of potential practical importance, (b) more efficient and more selective catalytic systems, and (c) new stoichiometric and catalytic reactions presently not possible with conventional catalysts. Our study of the chemistry of the lanthanide-carbon bond has led to the first molecules containing lanthanide-hydrogen bonds. These lanthanide hydrides catalytically activate molecular hydrogen and we are studying the intermediates in this reaction to understand how to modify this reactivity in unusual ways. The reactions of the hydrides with nitriles, isocyanides, alkynes and alkenes provide new, structurally unusual complexes whose chemistry is being examined. We have developed an efficient conversion of bimetallic hydrides to structurally unique trimetallic tetrahydrides which may be of interest with respect to hydrogen storage. We are studying the extension of this synthesis to larger polymetallic lanthanide polyhydrides.

UNIVERSITY OF COLORADO
Boulder, Colorado 80309

308. PROMOTER MODIFICATIONS OF CATALYTIC ACTIVITY AND SELECTIVITY — $145,000 24 mo. FY 82-83 — 02-01
John L. Falconer
Chemical Engineering Department

The influence of alkali promoters on CO hydrogenation is being studied as a function of catalyst support, promoter preparation method and promoter concentration. Temperature-programmed reaction is being used to measure specific rates of CO and carbon hydrogenation and temperature-programmed desorption is used to study changes in CO and H_2 desorption rates. The activity and selectivity to higher hydrocarbons is being studied in a differential reactor with gas chromatography detection. On all nickel catalysts, the selectivity to higher hydrocarbons, particularly olefins, was increased by the addition of Na or K promoters. For approximately one percent potassium and ten percent nickel, the specific activity decreased and the activation energy changed on Ni/TiO_2, Ni/Al_2O_3 and Ni/SiO_2. On $Ni/SiO_2 \cdot Al_2O_3$, however, specific activity increased. Good agreement was obtained between TPR and differential reactor studies. On Ni/SiO_2, the rate of carbon hydrogenation and the strength of hydrogen bonding also decreased with promoter addition. The method of promoter addition had a small influence on the activity and selectivity.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, California 93106

309. STUDIES RELATED TO THE HOMOGENEOUS CATALYSIS OF THE WATER GAS SHIFT REACTION — $66,500 — 02-01
Peter C. Ford
Department of Chemistry

Research in these laboratories is directed toward elucidating fundamental mechanisms key to catalytic cycles including the water gas shift reaction and toward developing new homogeneous catalysts for such reactions. Studies in progress include kinetic investigations of important steps such as the nucleophilic activation of carbon monoxide coordinated to metal centers by a variety of species including the oxy anions HO^- and CH_3O^- ($M\text{-}CO + RO^- \rightarrow M\text{-}CO_2R^-$), the decarboxylation of hydroxy carbonyl adducts ($M\text{-}CO_2H^- \rightarrow M\text{-}H^- + CO_2$), the reductive elimination of H_2 from metal hydrides ($M\text{-}H^- + H_2O \rightarrow H_2 + M + OH^-$) and the substitution reactions of metal carbonyl complexes. Systems under investigation are largely drawn from those shown to have potential as homogeneous catalysts in the reactions of carbon monoxide. The elucidation of these mechanisms will provide guidelines for the molecular engineering of new and better catalysts for the production of fuels and other organic products from CO and other small molecule substrates.

Chemical Energy, continued

CORNELL UNIVERSITY
Ithaca, New York 14853

310. ESR STUDIES OF SURFACE ADSORPTION AND CATALYSIS UNDER ULTRA-HIGH VACUUM CONDITIONS — $50,000 — 02-01
Jack H. Freed
Department of Chemistry

The objective of this project is the development of a new approach for the study of surface adsorption and catalysis on clean metallic and oxide surfaces by ESR spectroscopy. In the experiments performed in this project, the microwave cavity is itself part of the ultra-high vacuum (UHV) system, so that clean metallic surfaces are prepared by vacuum evaporation onto the interior of the cavity walls. Various clean gases are then directly adsorbed onto the surface and in situ ESR spectra are obtained which permit the study of paramagnetic adsorbates and surface reaction kinetics. These studies are complemented by simultaneous studies of the new phenomenon: CREMSEE (cyclotron resonance from microwave-induced secondary electron emission), which is also observed in the UHV-ESR microwave cavity and is found to be very sensitive to bonding of adsorbates to the metallic surface. By means of the Photo-CREMSEE technique, in situ work function measurements are also made to characterize the surface. New time-resolved ESR techniques will permit the study of fast surface reaction kinetics.

INDIANA UNIVERSITY
Bloomington, Indiana 47405

311. RADICAL CHAIN AND REARRANGEMENT REACTIONS IN COAL LIQUEFACTION — $68,000 — 02-01
Joseph J. Gajewski
Keven E. Gilbert
Department of Chemistry

This project focuses on providing fundamental data for the thermal reactions of aromatic compounds that may serve as a basis for understanding coal liquefaction. It has been shown that 1,3-diarylhydrocarbons and ethers decompose by free radical chain processes in the temperature range of 310 to 390°C. Some of these species will react with lower temperature free radical initiators and the kinetics and the thermodynamics of these reactions have been studied. Hindered phenols will inhibit radical chain reactions up to 200°C. We have also found that phenyl substituted tetralins cleave to smaller molecules via a complex series of radical rearrangements and phenyl shifts. Finally p-isotoluene and benzo-p-isotoluene, putative intermediates in the concerted retro-ene decomposition of 1,3-diphenylpropene, undergo thermal reactions with second order kinetics to give non-ene dimers and polymers respectively.

PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

312. MECHANISTIC STUDIES OF CARBON MONOXIDE REDUCTION — $72,000 — 02-01
Gregory L. Geoffroy
Department of Chemistry

Mechanistic schemes for the metal surface catalyzed reduction of carbon monoxide to methanol and to hydrocarbons have been proposed, and the feasibility of these mechanisms are being tested by preparing and studying the chemistry of metal clusters which resemble the proposed surface intermediates. Initial focus has been on the preparation and reactivity studies of cluster complexes bearing formyl and acyl substituent groups. The stepwise reduction of CO to CH_4 on an Os_3 cluster via a formyl intermediate had been observed. More recently it has been found that $Os_3(CO)_{11}(\mu\text{-}CH_2)$, an isolatable intermediate in the preceding transformation reacts readily with CO to yield the first ketene substituted cluster, $Os_3(CO)_{12}(\eta^2(C,C),\mu_2\text{-}CH_2CO)$. This species has been characterized spectroscopically and by a single crystal X-ray diffraction study and its chemistry is now being explored in detail. A series of mixed-metal dinuclear complexes have been synthesized and their CO/H_2 reactivity is being examined. Focus is on dinuclear complexes containing one early and one late transition metal and held together by bridging $\mu\text{-}PR_2$ groups.

Chemical Energy, continued

PENNSYLVANIA STATE UNIVERSITY
University Park, Pennsylvania 16802

313. THE NATURE OF THE CONTRIBUTION OF THE POLYMERS OF CELL WALLS OF THE HIGHER PLANTS TO COAL FORMATION — $50,000 — 02-01
Peter H. Given
Coal Research Section

The objective is to identify in peats the chemically altered forms of the plant polymers that constitute the input to coalification. Cores from four sites in the Florida Everglades and Okefenokee swamp have been obtained. About 30-50% of the organic matter in all levels of a peat derived from the red mangrove consists mostly of tissue from the rootlets and secondary roots of the tree. Specimens of these organs hand-picked from the upper layers of the peat show strong carbohydrate character, judging from FTIR and ^{13}C nmr spectra, but are not purely cellulosic. Nevertheless, the abundant rootlets from +40 mesh sieved material has a pronounced aromatic character, which resembles but is not identical with lignin, apparently because the rootlet material is encrusted with brown amorphous (humic?) substances. It has been found that oxidation with pertrifluoroacetic acid almost completely destroys cellulose but with lignin gives a good yield of a rather small number of simple polycarboxylic acids. The method has promise for the study of peats. In summary, the peat studied contains both carbohydrate- and lignin-related substances, but these are not identical with the natural polymers.

UNIVERSITY OF UTAH
Salt Lake City, Utah 84112

314. LIGAND INTERMEDIATES IN METAL CATALYZED CO REDUCTION — $163,604, 24 mo., FY 82-83 — 02-01
John A. Gladysz
Department of Chemistry

This research program has as its basic goal the synthesis and study of homogeneous complexes containing ligand types (-CHO, =CHOH, $=CH_2OH$, ≡C, ≡CH, $=CH_2$, $H_2C{=}O$, -OCHO, etc.) believed to be intermediate in the metal catalyzed conversion of CO/H_2 gas mixtures to organic molecules. Mechanistic understanding of the steps involved in catalytic CO reduction, and insight needed for the design of new catalysts, is sought. Current studies are making extensive use of optically active substrates derived from easily resolved $[(\eta\text{-}C_5H_5)Re(NO)(PPh_3)(CO)]^+ BF_4^-$. For instance, methylidene (+)-(S)-$[(\eta\text{-}C_5H_5)Re(NO)(PPh_3)(=CH_2)]^+ PF_6^-$ ((+)-(S)-1) couples to ethylene complex (+)-(R)-$[(\eta\text{-}C_5H_5)Re(NO)(PPh_3)(H_2C{=}CH_2)]^+ PF_6^-$ with retention. This coupling also exhibits a remarkable degree of enantiomer self-recognition: the (+)-(S)-1 couples virtually exclusively with (+)-(S)-1, and (-)-(R)-1 couples virtually exclusively with (-)-(R)-1. The formate (+)-(R)-$(\eta\text{-}C_5H_5)Re(NO)(PPh_3)(OCHO)$ decarboxylates at 70-130 °C to hydride (+)-(S)-$(\eta\text{-}C_5H_5)Re(NO)(PPh_3)(H)$ with retention. An X-ray structure study of $[(\eta\text{-}C_5Me_5)Re(NO)(P(OPh)_3)(=CH_2)]^+ PF_6^-$ has been submitted for publication.

UNIVERSITY OF UTAH
Salt Lake City, Utah 84112

315. LIQUID AND SOLID CARBON-13 MAGNETIC RESONANCE STUDY OF HYDROCARBONS AND RELATED SUBSTANCES — $90,026 — 02-01
David M. Grant, Dept. of Chemistry
Ronald J. Pugmire, Dept. of Fuels Engrg.

This work focuses on both liquid and solid NMR methods to characterize carbonaceous compounds important in the energy industry. The methods are being calibrated using model organic compounds. Hydroaromatics, coal macerals, various fossil fuels and their precursors provide the main focus of this work. A portion of this project has focused on the conformational analysis of hydroaromatics using liquid NMR methods. The effect of dipolar-dephasing and cross-polarization methods on quantitative measurements are being studied. 2-Dimensional Fourier techniques may be used to differentiate and distinguish different spectral responses in solids. The most useful portrayal involves a chemical shift versus scalar coupling plot. Presently, the data is obtainable on solids with reasonably high internal motion. The dipolar decoupling power used in proton decoupling is insufficient at present to provide scalar coupling constants for very rigid solids. Spreading spectral information into a second dimension helps resolve otherwise overlapping spectral responses. Thus, quantitative estimates of coal composition will be enhanced by this development.

Chemical Energy, continued

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

316. ORGANOMETALLIC CATALYSTS AND ANALOGS FOR CO REDUCTION AND CARBON-CARBON BOND CLEAVAGE REACTIONS
Robert H. Grubbs
Department of Chemistry

$188,000
24 mo.
FY 82683

02-01

The research is concerned with the activation and reduction of carbon monoxide. Group VI-B intramolecular metalloesters are synthesized from cationic transition-metal(II) carbonyl complexes employing intramolecular nucleophiles. Spectroscopic and X-ray crystallographic evidence confirm the general structure as an ester derived from the attack of an alkoxide at a carbonyl ligand. Equilibrium studies indicate that attack by an intramolecular nucleophile may be favored over that of an intermolecular one by at least four orders of magnitude. The optimum configuration for intramolecular nucleophilic attack is being investigated. One-electron electrochemical oxidation of an arene chromium carbonyl complex containing a pendant alcohol induces an interaction at bound CO. A family of Group IV ketene complexes have been synthesized as models for C-C coupling intermediates in CO reduction reactions.

YALE UNIVERSITY
New Haven, Connecticut 06520

317. SELECTIVITY ACTIVITY AND METAL-SUPPORT INTERACTIONS OF Rh BIMETALLIC CATALYSTS
Gary L. Haller
Department of Chemical Engineering

$75,000

02-01

This research program is designed to investigate the effects of a modifying second metal and/or the support on the selectivity and activity of Rh supported catalysts. A comparative extended X-ray absorption fine structure analysis of Rh-Ag/SiO_2 and Rh-Ag/TiO_2 indicates greater Rh-Ag interaction on the TiO_2 support than on SiO_2. This is reflected in the activity of structure sensitive reactions, e.g. hydrogenolysis, as a large decrease in activity as the Ag:Rh ratio is increased. The group VIII-TiO_2 support interaction behaves analogously to the group VIII-group 1b, e.g. Rh-Ag, interaction with respect to kinetic parameters and relative effect on structure sensitive vs. structure insensitive reactions. The kinetics of the group VIII-TiO_2 interaction indicate a transport limited process at a fixed reduction temperature. From these results we have deduced that group VIII-TiO_2 interaction involves transport of a reduced species, TiO_x, onto metal particles which break up large ensembles of surface metal atoms necessary to constitute sites for structure sensitive reactions.

UNIVERSITY OF CALIFORNIA/LOS ANGELES
Los Angeles, CA 90024

318. METALLACARBORANES STRUCTURALLY ENGINEERED FOR THE REDUCTION OF CARBON MONOXIDE
M.Frederick Hawthorne
Department of Chemistry

$70,000

02-01

This research program has been designed to develop and evaluate various metallacarboranes as homogeneous catalysts for the transformation of CO into useful chemical feedstocks. Emphasis has been placed on several areas of interest: (1) the evaluation of the activity of rhoda- and ruthenacarborane complexes as catalyst precursors for the water gas shift reaction; (2) the synthesis of heterobimetallic metallacarboranes which possess both early and late transition metal vertices, as well as those which contain main group elements such as aluminum and gallium, for the study of metal-metal cooperativity in the reduction of CO; and (3) the preparation and screening of a series of rhodacarborane complexes as hydroformylation catalysts. The ability to synthetically engineer the structural and electronic properties of metallacarboranes has proven to be an indispensible tool. The catalyst precursors used in these studies have been shown to exhibit several novel structural features which include a structurally sensitive closo/exo-nido tautomerism, a key feature in the ability of these species to activate small molecules such as dihydrogen.

Chemical Energy, continued

YALE UNIVERSITY
New Haven, Connecticut 06520

319. THE ROLE OF d-ELECTRONS IN CHEMISORPTION AND METAL/SUPPORT INTERACTIONS STUDIED BY ELECTRON SPECTROSCOPY
Victor E. Henrich
Applied Physics

$68,503
24 mo.
FY 82-83

02-01

This research program utilizes model supported catalysts (small Rh particles deposited in situ on well characterized TiO_2 single-crystal surfaces) and surface-sensitive electron spectroscopies, including photoemission and Auger spectroscopy, to examine the role of d-electrons and support electronic structure in strong metal/support interactions. Core level binding energies of the Rh atoms are found to depend upon particle size. The primary cause is believed to be changes in screening of the core hole, although changes in the valence state of the Rh atoms cannot be ruled out. Inert gas sputter profiling of model catalysts has shown that heating the catalyst to 400°C results in a decrease in the amount of exposed Rh, possibly by the coverage of Rh particles by an oxide of Ti. Changes in the chemisorption of CO and H_2 for various catalyst treatments are currently being investigated in order to correlate the electronic and geometric effects that have been observed to strong metal/support interactions.

UNIVERSITY OF PITTSBURGH
Pittsburgh, Pennsylvania 15260

320. STUDIES OF SUPPORTED METAL CATALYSTS
David M. Hercules
Department of Chemistry

$80,000

02-01

During this period we have advanced the adaptation of spectroscopic techniques for studying catalytic surfaces demonstrating the utility of ESCA, ISS and LRS. LRS can give structural information about bulk phases whereas ESCA can give information about highly dispersed phases. We have demonstrated a correlation between ESCA, EXAFS and PAS measurements, giving valuable information about the site symmetry of transition metals on catalyst surfaces. We have shown a correlation between reducibility of catalytic species measured by ESCA and the same quantity measured classically. We have characterized Ni species on Al_2O_3 and SiO_2 when the preparation method and Ni content of the catalysts are varied. We have studied the nature of Co species on Al_2O_3 and how they are affected by Mo or Zn, or by sulfiding. We have determined how Mo species on an alumina catalyst are affected by sulfiding, by the presence of Co or by being supported on titania. We have studied tungsten on alumina; the catalytic W species differ from Mo for the same support.

SRI INTERNATIONAL
Menlo Park, California 94025

321. HIGH TEMPERATURE CHEMISTRY OF COMPLEX VAPORIZATION/DECOMPOSITION PROCESSES
Donald L. Hildenbrand
Physical Sciences Division

$94,961

02-01

The objective of this program is to obtain fundamental thermodynamic data for a variety of high temperature vaporization/decomposition processes that are relevant to current and emerging energy technologies such as stack gas cleanup, coal gasification, hydrogen generation, and MHD. These processes are being studied by high temperature mass spectrometry and by the torsion-effusion method so that both vapor composition and absolute pressures are determined. For substances that simultaneously undergo both decomposition and direct vaporization, particular emphasis is on quantitative determination of the relative contributions from each process, and on thermochemical characterization of the complex vapor species. Current studies are concerned primarily with metal sulfate processes, with recent work on the sulfates of Cs, Rb, Fe, and Ni. The effects of certain additives that catalyze sulfate decomposition are also being studied, since kinetic and mechanistic features have a crucial bearing on the interpretation of the dynamic effusion measurements as well as on the technological applications of these processes.

Chemical Energy, continued

THE PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

322. CHARACTERIZATION OF ACTIVE SITES AND THEIR ROLE IN GAS-CARBON REACTIONS — $80,000 — 02-01
Robert C. Jenkins, Philip L. Walker, Jr. and Francis J. Vastola
Department of Materials Science & Engr.

This research is concerned with measuring the concentration of active sites on carbons varying in crystallite size and orientation (all the way from microporous carbons of poor crystallinity to natural graphite flakes of high crystallinity) and relating this concentration to gasification rates. Previous work has shown that the steady state gasification rate at 0.1 MPa O_2 correlates with the total amount of surface oxide and that CO can inhibit the steady state gasification rate. Current work is focused on characterizing the surface oxide formed during steady state gasification under varying conditions of temperature, pressure, and duration of reaction. The C-O_2 reaction is significantly catalyzed by Pt, e.g., the rate is about 400 times larger for 1% Pt deposited on a graphitized carbon black compared to the uncatalyzed case at 775 K and 0.1 MPa air. The reaction rates (673-773 K and 0.01 to 0.1 MPa O_2) are found to depend on the amount of Pt on the sample. The Pt dispersions on various samples are being determined by an x-ray line broadening and O_2-CO titrations at 298 K. The rate constants are found to be independent of average Pt dispersion.

UNIVERSITY OF ROCHESTER
Rochester, New York 14627

323. TRANSITION METAL ACTIVATION AND FUNCTIONALIZATION OF CARBON-HYDROGEN BONDS — $59,986 — 02-01
William D. Jones
Department of Chemistry

This research is directed towards the activation and cleavage of carbon-hydrogen bonds by homogeneous transition metal compounds. The possibilities for forming hydridometalaryl complexes and trapping these intermediates with isocyanides or acetylenes will be investigated. A reaction sequence involving trapping, insertion, and reductive elimination would yield imine or styrene products. These systems have the added feature that they can be catalytic, as the metal complexes are not consumed and the overall thermodynamics are favorable. The use of ω-arylacetylenes would permit the more facile intramolecular C-H activation, which would form fused ring systems if the proposed reaction sequence is followed. Metal complexes to be examined include $(C_5Me_5)RhL_2$, $(PR_3)_2ReH_7$, $(DMPE)_2TaH_5$, $H_5Ir(PMe_3)_2$, $Ru(PMe_3)_4$, $CpRe(PR_3)_2H_2$, $Mo(PMe_3)_4(N_2)_2$, and related molecules. The success of this project would result in a method for forming new carbon-carbon bonds.

OWENS-ILLINOIS, INC.
Toledo, Ohio 43666

324. INVESTIGATION OF SEMISYNTHETIC ESTERASES — $80,501 — 02-01
Melvin H. Keyes
Biotechnology Department

This research project is designed to study the nature of semisynthetic esterases, generated from nonesterase proteins, by means of conformational modifications induced by inhibitors of natural esterases. Two esterases are being generated from bovine pancreatic ribonuclease, using indolepropionic acid as the modifier, after perturbing the protein under acid pH and cross-linking with glutaraldehyde. The esterase activity is assayed using tryptophan ethyl ester as substrate and measuring the ethanol produced. The two esterases are distinguished by their distinct pH optima, substrate specificity and inhibition by tryptophan. After separation by ammonium sulfate precipitation, further purification of the esterases is being accomplished by gel filtration. The specificity of the esterases is being investigated using various esters, and amide substrates. Kinetic studies on the most appropriate substrates are being done.

Chemical Energy, continued

LEHIGH UNIVERSITY
Bethlehem, Pennsylvania 18015

325. MECHANISMS AND CONTROLLING CHARACTERISTICS OF THE CATALYTIC OXIDATION OF METHANE
Kamil Klier and Gary W. Simmons
Department of Chemistry
$210,000
24 mo.
FY 83-84
02-01

The objective of this program is to investigate the role of metal and oxide catalysts on the product composition in partial and full oxidations of methane. Studies of both the gas phase free radical pathways and the surface catalyzed reactions, as well as the interplay of the two, are incorporated in this program, using spectroscopic characterization of gas phase intermediates (EPR, optical) and of surface intermediates (Auger/ESCA/EELS). The gas phase and surface reactions occurring during partial oxidation of methane are being analyzed separately, and the program is divided into four tasks: 1. Trapping, Detection, and Identification of Free Radicals; 2. Electron Spectroscopy of Surface Intermediates: Auger/ESCA/LEED/TPD studies of halogen-treated palladium crystal surfaces; 3. Kinetic and Mechanistic Study of the Catalyzed Combustion of Methane; and 4. Effects of Nitric Oxide.

NORTHWESTERN UNIVERSITY
Evanston, Illinois 60201

326. SOLID STATE, SURFACE AND CATALYTIC STUDIES OF OXIDES
Harold H. Kung
Department of Chemical Engineering
$145,000
24 mo.
FY 83-84
02-01

This program is to elucidate the interrelation among the solid state, surface and catalytic properties of oxides. Current emphasis is on the effect of crystallite size and surface atomic structure in surface chemistry and catalysis. In the former, Fe_2O_3 catalysts of average crystallite sizes ranging from 2.5 to over 100 nm were prepared. Mössbauer, x-ray, and magnetization measurements indicated the presence of only α-Fe_2O_3. When used as catalysts for butene oxidation, the selectivity for butadiene was found to decrease from about 80% to less than 40% with increasing crystallite size. In the study of surface atomic structure effect, single crystal planes of (0001), $(10\bar{1}0)$, $(40\bar{4}1)$, and $(50\bar{5}1)$ of ZnO were used in the decomposition of methanol, formaldehyde, and formic acid. The product distributions on $(10\bar{1}0)$, $(40\bar{4}1)$ and $(50\bar{5}1)$ were the same but the decomposition activity increased with step density. The primary reaction is the oxidation to formate which decomposed into CO, CO_2, H_2 and H_2O. On the (0001) surface, in addition to oxidation, a dehydrogenation pathway also exists to yield formaldehyde, H_2 and CO from methanol.

TEXAS A&M UNIVERSITY
College Station, Texas 77843

327. CATALYSTS AND MECHANISMS IN SYNTHESIS REACTIONS
Jack H. Lunsford
Department of Chemistry
$93,579
02-01

A major part of this research program is devoted to understanding the structural and electronic factors which determine the catalytic properties of supported metals, such as palladium, for the formation of alcohols. Controlled modification of the support, for example by the addition of lithium ions, can transform an inactive catalyst into one which rivals commercial catalysts for methanol synthesis activity. Infrared experiments, using CO as a probe molecule, are underway to determine the relative amounts of Pd(111) and Pd(100) planes which are exposed on the supported catalysts. Another aspect of the research involves a study of matrix-isolated gas phase radicals which are produced on surfaces of catalytic importance. Recent work on magnesium oxide shows that surface defects which give rise to O^- ions (V-type centers) are active for the generation of methyl radicals from methane. These centers are present only on oxygen-rich surfaces which is surprising since magnesium oxide is normally considered to be a nonreducible oxide.

NATIONAL BUREAU OF STANDARDS
Washington, DC 20234

328. STRUCTURES AND REACTIVITY OF CHEMISORBED SPECIES AND REACTION INTERMEDIATES — $120,000 — 02-01
Theodore E. Madey, Richard D. Kelley

Surface Science Division

This program addresses the structure and reactivity of adsorbed molecules both on single crystal catalysts and high area catalysts using a variety of experimental methods. It involves four areas of research which have a common theme -- the investigation of surface processes related to catalytic chemistry. 1) The role of catalyst promoters and poisons in inducing new surface structures in molecular complexes adsorbed on metal and oxide surfaces is being studied using the electron stimulated desorption ion angular distribution (ESDIAD) method. 2) Vibrational spectroscopy of the adsorption, decomposition, and reaction kinetics of H_2O and NH_3 on single crystal metal and oxide surfaces is being studied using high resolution electron energy-loss spectroscopy (EELS). 3) Neutron inelastic scattering (NIS) is being used to characterize the vibrations of surface species on Raney Ni and Pt-black catalysts. The utility of NIS as an in situ probe of CO hydrogenation under reaction conditions has been demonstrated. 4) CO hydrogenation reactions over single crystal catalysts (refractory metals and Cu/Ni alloys) are under investigation.

STANFORD UNIVERSITY
Stanford, California 94305

329. MOLECULAR BEAM STUDIES OF THE DYNAMICS OF ACTIVATED ACTIVATED ADSORPTION OF N_2 ON W(110). — $218,504 — 24 mo. — FY 83-84 — 02-01
Robert J. Madix
Department of Chemical Engineering

The activated adsorption of N_2 on W(110) was studied using molecular beams to achieve translational energies from 2 to 30 kcal/gmol. The beams were formed in nozzles with and without helium seeding. For the lowest kinetic energy the probability of dissociation upon collision was about 10^{-3}, increasing to 2×10^{-1} at energies above 20 kcal/gmole. The dependence of the dissociation probability on nitrogen coverage suggested the process was direct in nature, not trapping dominated. The results show that adsorption is translationally activated and that the reactive collision is not adequately described by a one-dimensional barrier. As the beam energy was increased, the apparent saturation coverage by nitrogen increased, producing an unusual desorption state above a nitrogen atom coverage of 0.25. Nitrogen desorbed autocatalytically from this state in a fashion observed previously for high concentrations of oxygen from Pt(100). The emergence of this state at higher surface coverages indicates that the state of nitrogen adsorbed on tungsten and other metals may be quite different from the state normally observed in low pressure studies.

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

330. THE PHOTOCHEMICAL PROPERTIES OF TRANSITION METAL-ARENE COMPLEXES. — $72,448 — 02-01
Kent R. Mann
Department of Chemistry

The photochemical reactivity of transition metal arene complexes will be studied by examining the mechanisms of the arene replacement reactions by NMR, laser flash photolysis and classical mechanistic techniques. The intermediate species generated in these reactions will be utilized as catalytic photoassistance agents and in the synthesis of novel organometallic complexes.

Chemical Energy, continued

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, California 93106

331. REACTIONS OF IRON ATOMS WITH MOLECULES IN LOW TEMPERATURE MATRICES — $63,148 — 02-01
Ralph G. Pearson and Paul H. Barrett
Departments of Chemistry and Physics

The goal of this project is to study the reactivity of metal atoms and small clusters with molecules in low temperature matrices. Mössbauer and infrared spectroscopies are used to identify the reaction products. Reactions between Fe, Fe_2, and iron clusters and low temperature matrix isolated molecules of CO, C_2H_2, HCN, CH_4, CH_2N_2 and other small molecules are under investigation. This investigation includes the search for bond cleaving reactions of HX and CH_3X molecules and the study of CH_2, NH and O bound to iron atoms.

INDIANA UNIVERSITY-PURDUE UNIVERSITY
Indianapolis, Indiana 46223

332. STUDIES OF METAL-AMMONIA INTERACTIONS WITH AROMATIC SUBSTRATES — $47,000 — 02-01
Peter W. Rabideau
Department of Chemistry

Reduction and reductive alkylations effected by electron addition in dissolving metal systems such as sodium or lithium in liquid ammonia, can provide an important method for the solubilization of coal. This research is aimed at a better understanding of the fundamental nature of this reaction using aromatic and polynuclear aromatics as model compounds. The intermediates in these reactions are monoanions, radical anions and dianions, and efforts to study them involve direct and indirect methods. Direct studies include proton and carbon NMR with monoanions in liquid ammonia, whereas indirect studies involve determination of protonation sites (regioselectivity) and stereochemical outcome of alkylation. The conformational analysis of the reduced products (partially unsaturated six membered rings) is also being considered experimentally with proton and carbon NMR, as well as theoretically with force field calculations.

MARQUETTE UNIVERSITY
Milwaukee, Wisconsin 53233

333. POLYMER-BASED CATALYSTS — $105,000 24 mo. FY 82-83 — 02-01
Steven L. Regen
Department of Chemistry

This research is aimed at developing highly active and stable polymeric catalysts for use in aqueous/liquid organic two phase and aqueous/resin/liquid organic three phase reactions. Current effort is focusing on poly(ethylene glycols) and poly(ethylene glycol)-grafted copolymers as catalysts for promoting dehydrohalogenation, alkylation and saponification processes. Preliminary results indicate that significantly improved synthetic procedures are possible based on such catalysts, which should be amenable for a variety of laboratory as well as industrial applications.

UNIVERSITY OF NEBRASKA/LINCOLN
Lincoln, Nebraska 68588-0304

334. STUDIES ON UNUSUALLY REACTIVE METAL POWDERS. PREPARATION OF NEW ORGANO-METALLIC COMPOUNDS.
Reuben D. Rieke
Department of Chemistry

$90,000
18 mo.
FY 82-83

02-01

This research program is involved with the preparation and study of highly reactive metal powders prepared by the reduction of metal salts with alkali metals. Current studies are concentrating on nickel, cadmium, uranium, palladium, and platinum. The nickel powders have been found to react rapidly with benzylic halides and the resulting organonickel intermediate reacts with acid chlorides to yield benzyl ketones. Reactions of ROCOCOCl and benzylic halides with nickel powders yield dibenzyl ketones. These reactions proceed with a wide variety of substituents on the phenyl ring of the benzylic halides. Highly reactive uranium has been prepared and found to react with a variety of oxygen containing organic substrates such as nitrobenzene. Products are currently under investigation. Chemistry of cadmium, platinum, and palladium is also under investigation.

TEXAS A & M UNIVERSITY
College Station, Texas 77843

335. CATALYTIC BEHAVIORS OF MULTI-VALENT LANTHANIDE OXIDES
Michael P. Rosynek
Department of Chemistry

$131,193
24 mo.
FY 83-84

02-01

This research program involves a systematic investigation of the influence exerted by selected lanthanide oxide supports, principally those of La, Ce, Pr, and Eu, on the catalytic behaviors of both well-dispersed (Pt, Ir, Rh) and poorly-dispersed (Fe, Co, Ni) transition metals, with a view toward identifying evidence for significant metal-support interactions. Supports being studied as a basis of comparison include silica, alumina, and titania. Catalytic behaviors of the various metals are being evaluated for appropriate diagnostic reactions, viz., CO hydrogenation and paraffin hydrogenolysis/dehydrocyclization, as a function of conditions and support identity. These results are being correlated with those of accompanying characterization studies, involving infrared and x-ray photoelectron spectroscopies, transmission and scanning electron microscopies, electron microprobe analyses, and selective chemisorption measurements, in an attempt to elucidate the nature and extent of metal-support interaction effects.

UNIVERSITY OF KENTUCKY
Lexington, Kentucky 40506

336. FUNDAMENTAL STUDY OF CATALYSTS USING LASER RAMAN, INFRARED, AUGER ELECTRON SPECTROSCOPY AND LOW ENERGY ELECTRON DIFFRACTION
G. A. Sargent, Dept. of Met. Engr.
E. B. Bradley, Dept. of Elec. Engr.

$70,000

02-01

The goal of this project is to develop an understanding of catalytic activity and selectivity with the long-range goal of producing better catalysts. The techniques of LEED, Auger spectroscopy, and laser Raman and infrared spectroscopies are used to study the surface structure and bonding of CO, CH_4, H_2 and O_2 adsorbed on Ni(111) and Ni(100) single crystal surfaces. The surface coverage was controlled by varying the gas pressure and exposure time. Surface dipoles (magnitude and orientation) are measured for each gas adsorbed on the surface by a combination of work function change measurements and spectroscopic techniques. Laser Raman and infrared spectroscopy are used to determine vibrational modes of surface structures of the adsorbed molecules and the polarization of Raman bands. Changes in band intensities are used to measure electric dipole orientation and thermal desorption characteristics. Thermal desorption experiments have been undertaken for each gas adsorbed on each surface using the linear temperature programming technique. The mass of the desorbed species is determined by a precision mass analyzer. The mass analyzer is also used to determine residual gas concentrations in the experimental chamber and to identify the structure of intermediate molecules.

Chemical Energy, continued

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts 02139

337. REDUCTION OF CARBON MONOXIDE — $215,000 — 24 mo. — FY 83-84 — 02-01
Richard R. Schrock
Department of Chemistry

The object of this research is to learn how to reduce carbon monoxide catalytically and selectively to a two-carbon product such as ethanol, ethylene glycol, ethylene, or acetaldehyde. The approach is to discover how earlier transition metal hydride complexes can take part in unique reactions not possible with the later transition metals; i.e., what new principles of catalytic reduction of carbon monoxide remain to be discovered. The program involves the synthesis of new transition metal hydrido complexes and a detailed study of how they react with carbon monoxide. The program began with a study of a new dimeric tantalum hydrido complex which reacted with the carbon monoxide to give a μ-hydrido μ-formyl species. Analogous reactions employing metals which are less oxophilic are being sought. At present we are investigating some novel tungsten hydrido clusters and complexes containing linked cyclopentadienyl ligands including a late/early transition metal combination. The late/early transition metal complex is being tested for activity under typical syngas conditions.

PENNSYLVANIA STATE UNIVERSITY
University Park, Pennsylvania 16802

338. ORGANOMETALLIC CHEMISTRY OF WEAKLY SOLVATED TRANSITION METAL CATIONS — $115,000 — 24 mo. — FY 82-83 — 02-01
Ayusman Sen
Department of Chemistry

The present research is concerned with the rational design of transition metal compounds which may be used as homogeneous catalysts for organic and polymer synthesis. The approach that we have developed is to synthesize transition metal cations incorporating weakly coordinating solvent molecules which dissociate readily, thus allowing substrates to enter and react within the coordination sphere of the metal. Thus far, using this approach, we have successfully synthesized an entirely new class of metal complexes which are versatile catalysts for the polymerization, linear and cyclic oligomerization and rearrangement of a wide range of olefinic substrates, as well as the linear polymerization of acetylenic substrates containing both electron-withdrawing and electron-donating substituents. In addition, we have discovered the first catalysts for the room temperature copolymerization of carbon monoxide with olefins. The resultant polyketones constitute a new class of materials which are expected to have properties such as photo- and bio-degradability.

NORTHWESTERN UNIVERSITY
Evanston, Illinois 60201

339. STRUCTURE AND CHEMISTRY OF THE INTERACTION OF ORGANOMETALLICS WITH SURFACES — $90,000 — 02-01
Duward F. Shriver
Department of Chemistry

The objective of this research is to characterize organometallics attached to surfaces. The primary techniques include quantative analysis of gases evolved upon interaction of the organometallic with the surface, fourier transform infrared spectroscopy, Raman spectroscopy, and extended X-ray absorption fine structure. Initial studies will center on metal carbonyls attached to metal oxide surfaces. Parallel studies will be performed on molecular compounds which simulate the proposed surface species. Catalytic activity of some of the surface organometallics will be investigated.

Chemical Energy, continued

COLORADO STATE UNIVERSITY
Fort Collins, Colorado 80523

340. REACTIONS OF ALKYL PALLADIUM AND PLATINUM DIMERS. MECHANISMS OF DINUCLEAR ELIMINATION — $65,000 — 02-01
J. K. Stille
Department of Chemistry

Metal Clusters can serve as models for metal surfaces in catalysis, and because the cluster is well defined and amenable to study by the methods and techniques available to homogeneous systems, the reactions on clusters can be studied in detail. Thus, a knowledge of the mechanisms of reactions that occur on clusters can provide a better understanding of heterogeneously catalyzed reactions and help in developing new heterogeneous catalysts. The synthesis of dinuclear platinum, palladium and rhodium complexes containing organic groups on adjacent bonded metals, and the reactions of these complexes, particularly the 1,2-reductive elimination rearrangement, oligomerizations and insertion reactions are being carried out. Elucidation of the mechanism(s) of these reactions should provide a better understanding of how coupling, oligomerization and isomerization reactions of hydrocarbons take place on metal surfaces.

UNIVERSITY OF CHICAGO
Chicago, Illinois 60637

341. THE REACTIONS OF ELECTROPHILIC REAGENTS WITH BITUMINOUS COALS. THE CHEMISTRY OF THE REACTION PRODUCTS. — $81,061 — 02-01
Leon M. Stock
Department of Chemistry

The electrophilic reactions of bituminous coals are under investigation. Preliminary reactions with mercury (II), lead(IV) and ruthenium(VIII) have been carried out.
The plumbylation reaction of Illinois No. 6 coal yields a product which undergoes oxidative solvolysis to yield a material selectively enriched in aryl hydroxyl groups. The preliminary results suggest that this altered coal undergoes donor solvent liquefaction in tetralin to yield a product which is less soluble in pyridine but more soluble in hexane than the natural material.
The preliminary results of selective catalytic oxidations with ruthenium(VIII) are also most encouraging. Illinois No. 6 coal undergoes oxidation in 2 hours at ambient temperature in neutral solution in the presence of catalytic quantities of ruthenium(III) and an excess quantity of a cooxidant such as sodium periodate or sodium hypochlorite. About 225 different soluble carboxylic acid ester compounds are formed in the reaction.

THE PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

342. METAL-SUPPORT INTERACTIONS IN Ni, Pd, and Pt CATALYSTS — $81,564 — 02-01
M. Albert Vannice
Department of Chemical Engineering

This research proposal is directed toward a better understanding of the chemistry involved in the creation of metal-support interactions in certain systems, which have been found to have pronounced effects on adsorption and catalytic behavior. This is presumed to be due to modifications of the adsorbed state of reactant molecules, and this program involves a study of heats of adsorption and desorption energies for H_2, CO, and O_2 on Pt, Pd, and Ni using a modified differential scanning calorimeter and a thermal gravimetric analysis unit. Separate chemisorption experiments are being conducted in a volumetric adsorption system, and kinetic investigations being made on the hydrogen of carbon monoxide and aromatic hydrocarbons, beginning with benzene. Possible correlations between catalytic activity and adsorbate-metal bond strengths are being investigated. This multifaceted approach should provide a more complete explanation of both the much higher catalytic activities already found in certain reactions and the suppressed chemisorption which is observed after the SMSI state is induced. The possibility that special active sites are created at the metal-support interface is also being carefully examined.

Chemical Energy, continued

YALE UNIVERSITY
New Haven, Connecticut 06511

343. ENERGIES OF ORGANIC COMPOUNDS — $80,000 — 02-01
Kenneth B. Wiberg
Department of Chemistry

This research program is designed to provide information on the energies of organic compounds via reaction calorimetry and theoretical calculations, and to use these data to improve empirical and semi-empirical schemes for estimating energies of these compounds. The data also are being used to explore steric effects and other structural effects on energies. Reactions being studied include the hydration of alkenes, hydrolysis of ketals, reduction of ketones, and rearrangements of small ring hydrocarbons. Theoretical calculations (RHF) are being used to estimate energies of interesting compounds which have not as yet been prepared, and to obtain charge distributions which are needed in the semi-empirical calculations.

SRI INTERNATIONAL
Menlo Park, California 94025

344. ADSORPTION THERMODYNAMICS AND SURFACE TRANSPORT OF METAL CATALYSTS POISONS — Total $71,997 — 02-01
Henry Wise and Jon McCarty
Materials Research Laboratory

This research has for its objective a fundamental understanding of the binding energy of sulfur and halogen adatoms to metal surfaces in order to relate catalysts poisoning and reactivation to covalent bond formation. The experimental measurements involve studies of equilibrium adsorption and surface diffusion on single crystals of different orientations and on highly dispersed metal catalysts. The techniques employed include classical studies of reversible adsorption at low surface coverages, Auger electron spectroscopy for diffusional transport, and low energy electron diffraction for determination of surface coordination and reconstruction.

UNIVERSITY OF PITTSBURGH
Pittsburgh, PA 15260

345. INFRARED STUDIES OF THE INFLUENCE OF ALKALI METALS ON THE C-O BOND IN CHEMISORBED CARBON MONOXIDE — $186,555 19 mo. FY 82-83 — 02-01
John T. Yates, Jr.
Department of Chemistry

This research program is designed to probe the interaction of adsorbed alkali metals with adsorbed carbon monoxide on transition metal single crystal surfaces. Information obtained by Reflection IR Spectroscopy, X-Ray Photoelectron Spectroscopy, and Temperature Programmed Desorption will yield models of the interaction, and deeper understanding of the alkali promotion effects observed in catalytic chemistry on transition metals.

Chemical Energy, continued

ROCKWELL INTERNATIONAL
Canoga Park, California 91304

346. MOLTEN SALT INTERACTIONS IN COAL PROCESSING — $160,000 — 02-01
S. J. Yosim and G. B. Dunks
Energy Systems Group

This research program is designed to develop an understanding of the fundamental chemical and physical processes involved in the oxidation of carbon in molten salt media. The current investigation is directed toward determining the effect of sulfur (a major constituent of coal) on the oxidation process. Electrochemical techniques are being employed to determine the effects of melt temperature and sparge gas composition on the in situ concentrations of the chemical species (potential oxidants) which exist in mixed beds of sodium carbonate and sodium sulfate sparged with mixtures of oxygen, carbon dioxide, and nitrogen between 900-1000°C. Changes which occur in the concentrations of the melt species and in the composition of the exhaust gas as a function of time after the addition of graphite to the melt together with subsequent changes which occur as oxidation of the graphite proceeds to completion are being evaluated. The results of these studies are providing information concerning the identity of transient melt species, the mechanisms through which they are formed and the mechanisms through which they are consumed during graphite oxidation.

Separations and Analysis

UNIVERSITY OF TENNESSEE/KNOXVILLE
Knoxville, Tennessee 37996

347. SYSTEMATIC AND STRUCTURAL STUDIES OF POLYMERIC EXTRACTANTS FOR THE SEPARATION AND RECOVERY OF METAL IONS — $46,?13 — 02-02
Spiro D. Alexandratos
Department of Chemistry

The research is directed towards the synthesis and evaluation of polymer-supported extractants with emphasis on the properties of the polymeric support. In focusing on the development of polymeric extractants which will be commercially viable for large-scale applications to the recovery of strategically important metals and within nuclear waste reprocessing plants, the study is concerned with four major points: (1) develop an economical synthesis of the polymer support, (2) utilize polymers which display high chemical, mechanical, and radiation stability, (3) develop polymers with macroscopic properties allowing for a rapid rate of metal ion complexation, and (4) produce polymeric extractants with a high density of active sites in order to minimize bed volumes. The principle polymer support examined to date is polystyrene, in bead form, at various levels of crosslinker and macroporosity. Bonding phosphinic acid moieties to the styrenic network yields a polymer-supported extractant which is found to absorb large levels of metal ions from aqueous solutions even at low pH values.

Separations and Analysis, continued

UNIVERSITY OF MARYLAND
College Park, Maryland 20742

348. NON-DESTRUCTIVE DETERMINATION OF TRACE ELEMENT CONCENTRATIONS — $107,000 — 02-02
D. L. Anderson, G. E. Gordon, W. B. Walters, and W. H. Zoller
Department of Chemistry

A low background thermal neutron-base facility has been constructed at the National Bureau of Standards (NBS) reactor for the purpose of elemental analysis in various matrices. Samples of masses of 10 mg to 2 g are placed in the beam and the prompt γ rays (0.1-11.0 MeV) are measured. The elemental concentrations of H, B, C, N, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Mn, Fe, Cd, Sm and Gd can be determined in many materials. The method is capable of measuring all major elements (except O) in most types of samples. Present studies include standardizing PCBs for Cl content, accurately measuring boron in scintered pellets used as burnable poisons in the startup cycle in power reactors, and the characterization of a number of USGS, NBS and IAEA geological and biological standards. Another study concerning the fate of boron in coal-burning is underway. Experiments using ^{252}Cf as a neutron source for a laboratory-based prompt-γ facility continue.

UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

349. CONTINUOUS REACTION CHROMATOGRAPHY — $60,000 — 02-02
R. Aris
R. W. Carr
Department of Chemical Engineering and Materials Science

Continuous reaction chromatography is a method for carrying out chemical reaction with simultaneous chromatography of reactants and products in a single continuous flow reactor. This can be accomplished by providing relative motion between the chromatographic packed bed and the feedstream. Investigations of the rotating cylindrical annulus for both liquid phase reaction - solid adsorbent and gas - solid catalytic reactions have been completed. Also, a detailed modelling study of the behavior of a countercurrent moving bed chromatographic reactor has been done. Experimental tests of a laboratory scale countercurrent moving bed reactor are being carried out. Analysis of reaction products is being done by conventional gas chromatography. Reactor performance is being compared with theoretical predictions.

Separations and Analysis, continued

BEND RESEARCH, INC.
Bend, Oregon 97701-8599

350. FUNDAMENTALS OF COUPLED-TRANSPORT MEMBRANES — $91,786 — 02-02
Walter C. Babcock
Membrane Separations Division

The program objective is to study the fundamentals of coupled-transport membranes as applied to uranium separations. Coupled-transport membranes consist of a water-immiscible, liquid complexing agent held by capillary forces in the pores of a microporous polymeric support. This membrane separates two aqueous solutions of unequal concentrations. The complexing agent can pick up ions on one side of the membrane and carry them across the membrane by diffusion in the form of a neutral complex. Metal ions can be transported from a dilute to a concentrated solution by coupling their flow to that of another ionic species. The membranes are also selective due to the selectivity of the complexing agent toward uranium over other metals. Thus, coupled transport is of potentially practical value in hydrometallurgy and in the treatment of radioactive wastes. Current efforts are focused on studying long-term performance of the membranes. The goal is to overcome problems of limited lifetime that are common with these membranes. Substantial progress has been made in developing a predictive model for the development of membranes with commercially practical lifetimes.

UNIVERSITY OF MASSACHUSETTS/AMHERST
Amherst, Massachusetts 01003/0035

351. DYNAMICS OF, AND HEAT AND MASS TRANSFER IN, AN INDUCTION PLASMA — $60,000 — 02-02
Ramon M. Barnes
Department of Chemistry

This investigation involves the computer modeling and experimental verification of the inductively coupled plasma discharge operated at atmospheric pressure in argon and molecular gases. Calculation of flow and temperature fields for two major types of induction torches has been achieved with a new model using a velocity-pressure-temperature approach which has resulted in increased speed of convergence and stability. Conditions were simulated that were not possible with previous models. For argon and nitrogen discharges at 3 MHz, flow and temperature fields have been calculated for power levels between 5 and 20 kW and for central flows of 0 to 7 liter per minute. For spectrochemical torches at 0.75 kW, similar calculations were performed for frequencies between 13 and 40 MHz. In another calculation, flow and temperature fields were obtained including plasma particle interactions, especially heating loading effects and some changes of thermodynamic properties with vapor. Heavy loading of the 3 MHz plasma with up to 10 g/min Cu particles cooled the plasma, and extensive evaporation was observed with 40 micrometer particles. For alumina particles and water droplets only heat loading was considered. The particle interaction in the spectrochemical torch is being studied.

TEXAS TECH UNIVERSITY
Lubbock, Texas 79409

352. METAL ION COMPLEXATION BY IONIC CROWN ETHERS — $112,500 — 21 mo. — FY 83-84 — 02-02
Richard A. Bartsch
Department of Chemistry

The goals of this research are the synthesis of lipophilic crown ethers with pendant ionizable groups and the application of these compounds for selective metal ion complexation. A variety of lipophilic crown ether carboxylic acids are being prepared in which the following structural features are systematically varied: a) the size of the polyether cavity; b) the number and types of ethereal oxygens in the crown ether ring; c) the attachment site(s) for lipophilic groups; and d) the presence or absence of aromatic groups as polyether ring substituents. The first crown ether phosphonic and sulfonic acids are also being prepared. The efficiencies and selectivities of these lipophilic ionizable crown ethers in competitive solvent extraction, liquid surfactant (emulsion) extraction, and bulk liquid membrane transport of alkali and alkaline earth cations are being assessed.

Separations and Analysis, continued

AMHERST COLLEGE
Amherst, Massachusetts 01002

353. ISOTOPE EFFECTS IN THE SOLUTION OF GASES IN LIQUIDS — $47,080 — 02-02
Bruce B. Benson
Daniel Krause, Jr.
Department of Physics

The broad purpose of this research is to explore molecular interactions in dilute solutions of gases in liquids, especially water, by measuring the dependence of gas solubility on the isotopic masses of the solute and solvent. Measurements on the noble gases dissolved in H_2O have shown how the isotopic fractionation depends upon temperature, isotopic mass, and gas polarizability. Similar studies are being carried out on noble gas clathrate hydrates, in which the molecular structure of the hydrate is well known from x-ray analyses. A better understanding of the hydrogen bonded structure in liquid water may be obtained from a comparison of the extrapolations to 0°C of the results for the hydrates and liquid water. Gas solubilities in D_2O are being determined for comparison with previous results in H_2O

STATE UNIVERSITY OF NEW YORK, STONY BROOK
Stony Brook, New York 11794

354. FUNDAMENTAL STUDIES IN ISOTOPE CHEMISTRY — $98,000 — 02-02
Jacob Bigeleisen
Department of Chemistry

Experimental and theoretical investigations are made of isotope effects in chemical and physical processes. When appropriate, applications are made to isotope separation processes and nuclear fuel cycles. Calculations have been made of the expected chemical properties of super-heavy isotopes of hydrogen, carbon, selenium and uranium as a guide in the search for such particles. Detailed calculations have been made of the separation expected of superheavy isotopic forms of CO by fractional distillation. Relations between the isotope chemistry of oxygen and molecular structure are being studied. Regularities are found by an analysis of the effect of isotopic substitution on the entropies and enthalpies of formation of the compound from the gaseous oxygen atom.

BRIGHAM YOUNG UNIVERSITY
Provo, Utah 84602

355. SEPARATION OF SELECTED CATIONS BY LIQUID MEMBRANES — $64,754 — 02-02
James J. Christensen
Department of Chemical Engineering
Reed M. Izatt, Department of Chemistry

Macrocycle-mediated cation transport using bulk, emulsion, and lipid vesicle liquid membrane systems is being investigated and modeled. In water-halocarbon-water bulk liquid membranes, proton coupled transport of alkali metal ions from two, three, and four cation mixtures is being studied using calixarene macrocycles as carriers. The relative fluxes of cations from cation mixtures in water-toluene-water emulsion membrane systems is under investigation using the carrier dicyclohexano-18-crown-6 and various complexing anions in the interior receiving phase. The transport in these emulsion systems of amphoteric metals as anionic species coupled to a pH gradient across the membrane is also being studied. Dicyclohexano-18-crown-6 is being incorporated into phospholipid vesicles as a means of making them selectively permeable to cations. The chemical and thermodynamic characteristics of the interaction of Pb^{2+} with these vesicles is being investigated.

Separations and Analysis, continued

UNIVERSITY OF CALIFORNIA/LOS ANGELES
Los Angeles, California 90024

356. MULTIHETEROMACROCYCLES THAT COMPLEX METAL IONS — $125,000 — 02-02
Donald J. Cram
Department of Chemistry

This research involves the design, synthesis and evaluation of cyclic and multicyclic organic compounds that selectively complex metal salts and solubilize them in organic solvents. Spherands are synthetic ligand systems that in the uncomplexed state contain enforced cavities lined with electron pairs. Rigid cyclic frameworks support attached heteroelements so their unshared electron pairs possess a convergent arrangement. Spherands are being studied whose cycles are composed of six to eight six-membered rings bonded to one another at their 1,3-positions, and carrying substituents in their 2-positions. Chorospherands are part crown and part spherand, and cryptospherands are part cryptand and part spherand. Spherands, chorospherands and cryptospherands are being studied which contain anisyl, pyridine, pyridine oxide, benzoquinone, thioanisyl, cyclic urea and benzenecarboxamide units. Metal ion and isotope-specific complexing agents are being sought.

BROWN UNIVERSITY
Providence, Rhode Island 02912

357. PHOTOCHEMICAL GENERATION OF THE OPTO-ACOUSTIC EFFECT — $58,386 — 02-02
Gerald J. Diebold
Department of Chemistry

Research is being conducted into photochemical generation of the optoacoustic effect. The frequency, phase shift and amplitude dependence of the acoustic signal in nonlinear systems such as Cl_2 are being experimentally investigated. The effects of chemical inhibitors on the optoacoustic effect is also under investigation. The recently discovered chemical amplification of optoacoustic signals in chain reacting nonlinear systems is being extended to other photochemical systems that should be inherently linear. This should further establish the optoacoustic effect as a sensitive probe of photochemically generated exothermic reactions. In addition, a total internal reflectance optoacoustic effect is being studied for possible application as a spectroscopic or a trace detection method for gas phase species and bulk materials.

UNIVERSITY OF UTAH
Salt Lake City, Utah 84112

358. FOURIER TRANSFORM PHOTOACOUSTIC SPECTROSCOPY — $75,000 — 02-02
Edward M. Eyring
Department of Chemistry

Opaque solids of high surface area are being examined by Fourier transform infrared photoacoustic spectroscopy (FT-IR/PAS). Novel dopants (such as coordinative molybdenum and chromium carbonyls and trimethyloxonium salts) alter band gaps in electroconductive polymers such as polyacetylene, polyparaphenylene and their derivatives. Resulting infrared spectra are correlated with X-ray photoelectron spectra, solid state nuclear magnetic resonance spectra, and other spectral data to define the structure and reactivity of these materials. Multi-technique surface studies of high surface area heterogeneous catalysts such as sulfided Co-Mo/Al_2O_3 are also underway. Sample surfaces are selected for their properties that challenge the present capabilities of FT-IR/PAS and that force improvements such as photothermal beam deflection spectroscopy now also used in this laboratory.

Separations and Analysis, continued

PURDUE UNIVERSITY
West Lafayette, Indiana 47907

359. REACTIONS OF METAL IONS AND THEIR CLUSTERS IN THE GAS PHASE USING LASER IONIZATION-ION CYCLOTRON RESONANCE SPECTROSCOPY — $82,127 — 02-02
Ben S. Freiser
Department of Chemistry

A laser ionization source is used in conjunction with ion cyclotron resonance spectroscopy to generate and study the gas phase chemistry of simple metal ions and their clusters. Using this technique metal ions are generated directly by focussing a high-powered pulsed laser onto the pure metal. The goals of this work have been 3-fold: determination of fundamental reaction mechanisms and trends in reactivity; comparison of gas phase to solution phase results; and development of metal ions as selective chemical ionization reagents. These goals have been pursued thus far in extensive studies of Cu^+ with esters and ketones, on Fe^+ with ethers and ketones, and on Fe^+, Ti^+, Co^+, Ni^+, Rh^+, V^+, Y^+, and Sc^+ with hydrocarbons. In addition work has been started on the effect of ligands on metal ion reactivity. Studies of $M\text{-}X^+$ ions, where X=O,S, CH_2, CH_3, and C_2H_4, for example, are well underway. This work has been catalyzed further with the acquisition of a Nicolet Fourier transform mass spectrometer (FTMS). Of particular importance is the application of collision-induced dissociation using FTMS to elucidate ion structures and reaction mechanisms.

UNIVERSITY OF ARIZONA
Tucson, Arizona 85721

360. CHELATING EXTRACTANTS OF IMPROVED SELECTIVITY — $74,286 — 02-02
Henry Freiser
Department of Chemistry

This research is designed to develop chelating extractants of improved selectivity for separating individual lanthanide and actinide ions. Emphasis is being placed on uncovering molecular structural parameters of importance in the design of such extractants. Use of pattern recognition techniques represent one approach to the elucidation of molecular parameters. Study of the extraction equilibria for representative tervalent lanthanides with selected members of chelating extractants of the N-acylphenylhydroxylamine, 8-quinolinol, and acylpyrazolone families is being used both because they include some likely candidate extractants and because present gaps in fundamental data required to apply pattern recognition is thereby being acquired.

UNIVERSITY OF MISSOURI
Rolla, Missouri 65401

361. AN EXTRACTION/SEPARATION PROCESS WITH EXTREME ENERGY EFFICIENCY — $63,564 — 02-02
S. E. Friberg and P. Neogi
Department of Chemistry

The purpose of this investigation is to examine the phase equilibria involved in an extraction/separation process with extremely low energy demand. The process uses the temperature dependent transitions of colloidal association structures in systems of water/polyethylene glycol dodecyl ethers/ aliphatic hydrocarbons to permit spontaneous extraction and separation with a temperature change of only 20°C. The main emphasis is placed on the role of liquid crystals to influence the kinetics of the extraction process.

Separations and Analysis, continued

UNIVERSITY OF VIRGINIA/CHARLOTTESVILLE
Charlottesville, Virginia 22901

362. THE GLOW DISCHARGE AS AN ATOMIZATION AND IONIZATION SOURCE — $73,002 — 02-02
W.W. Harrison
Department of Chemistry

This project centers about the study of a glow discharge as an atomization and ionization source for trace element analysis of solids and solutions. Coupling of the glow discharge to a quadrupole mass filter results in a simple mass spectrometer system of considerable versatility. A variable duty pulsed discharge is being studied and shows advantages over direct current operation. The use of short, high intensity pulses produces enhanced sputter action and a greater ion yield. Time-resolved selection of ions generated only during the trailing pulse edge produces a strong atomic signal for the cathode sample with discrimination against background gases. The use of laser enhanced ionization within the glow discharge is also under investigation.

THE AEROSPACE CORPORATION
El Segundo, California 90245

363. LASER FLUORESCENCE STUDIES OF METALLIC IONS IN FLAMES FOR IMPROVED DETECTION — $95,000 18 mo. FY 82-83 — 02-02
F. E. Hovis and J. A. Gelbwachs
Chemistry and Physics Laboratory

The use of fluorescence methods on neutral metal atoms in flames is a well established analytical technique. We propose to investigate laser induced fluorescence of metallic ions in high temperature flames for analytical applications. The first study involves the direct laser excitation of ionic fluorescence of the alkaline earth metals. A second experiment investigates neutral-ion energy transfer in metals as a means of sensitized ion fluorescence for multielement analysis. The use of sensitized ion fluorescence would allow simultaneous analysis of several metals using a single laser excitation line. The use of neutral-ion energy transfer is anticipated to yield superior detection limits to neutral-neutral energy transfer and to have good potential as a practical analytical tool. These studies will yield information of both practical and fundamental interest.

THE UNIVERSITY OF WYOMING
Laramie, Wyoming 82071

364. SOLID SURFACE LUMINESCENCE ANALYSIS — $76,840 — 02-02
Robert J. Hurtubise
Chemistry Department

The main goal of this project is to develop a fundamental understanding of the physical and chemical interactions that induce strong room-temperature fluorescence and phosphorescence from organic compounds adsorbed on solid surfaces. Reflectance, infrared, nuclear magnetic resonance, and luminescence spectroscopy are being used to clarify the interactions. Luminescence polarization, and fluorescent and phosphorescent lifetime experiments are also being performed. The interactions in the initial wet solid-surface chemistry and their influence on the final luminescent signals in the dried solid matrix are being investigated. Experiments are being carried out to determine if the organic molecules are being held rigidly or if the solid matrix is preventing collisions with oxygen and water molecules. Basic and nonbasic nitrogen heterocycles and hydroxyl aromatics are being used as model compounds to develop total luminescence derivative spectroscopy as a new approach in organic trace analysis.

Separations and Analysis, continued

STATE UNIVERSITY OF NEW YORK/STONY BROOK
Stony Brook, New York 11794

363. STABLE ISOTOPE STUDIES — $108,370 — 02-02
Takanobu Ishida
Department of Chemistry

This project consists of basic studies of isotope effects (IE) and developmental investigations of methods for fractionating stable isotopes. A new mathematical method for directly correlating the zero-point energy (ZPE) to the forces and structures of molecules is applied to the ZPE of n-paraffins and the hydrogen/deuterium (H/D) IE in the ZPE of n-paraffins and halogen and oxygen compounds. A stainless steel packed column system is operated to determine ^{15}N separation characteristics of nitric oxide/dinitrogen trioxide process under pressures up to 15 atm. and temperatures between -15°C and 20°C. An electrochemical refluxer for the Nitrox ^{15}N separation process is developed to eliminate needs for chemical feeds and chemical waste disposal. Catalytic isotope exchange reactions between ammonia and hydrogen are studied. The $^{12}C/^{13}C$ and H/D vapor pressure isotope effects (VPIE) in liquid methlene difluoride and the $^{14}N/^{15}N$ and H/D VPIE in liquid and solid ammonia are measured using a differential manometry in a cryostat having a temperature stability and uniformity of one millidegree.

SAN DIEGO STATE UNIVERSITY
San Diego, California 92182

366. DEVELOPMENT AND OPTIMIZATION OF METHODOLOGIES FOR ANALYSIS OF COMPLEX HYDROCARBON MIXTURES — $60,000 — 02-02
R. J. Laub
Department of Chemistry

The goals of this project comprise exploration and further clarification of optimization methodologies for gas- and liquid-chromatographic separations of complex hydrocarbon mixtures. Emphasis is being placed at present on the kinetics of mass transfer, temperature effects, and mobile-phase composition in microbore-, conventional-bore, and rotating-disk thin-layer liquid-chromatographic techniques with silica, reversed-phase silica, and alumina adsorbents. Also being studied are metal-modified silica LC packings, including in situ generation and alteration of the adsorbent surface. The utility of binary carriers in gas chromatography is being examined, where the second-interaction virial coefficients are predicted in advance from the McGlashan-Potter equation. Solute retentions are then calculated, where the separations achieved are a function both of the carrier pressure and composition. Work on establishment of a standard set of stationary phases for gas chromatography is being continued, where emphasis is being placed on newly-synthesized mesomorphic polysiloxane (MEPSIL) solvents.

University of Georgia
Athens, Georgia 30602

367. A Study of Mechanisms of Hydrogen Diffusion in Separation Devices — $101,521 — 18 mo. — FY 82-83 — 02-02
M. Howard Lee
Department of Physics and Astronomy

This study centers on separating hydrogen from mixtures of light gases by means of diffusion through metals. The hydrogen diffusion is highly selective, showing nonclassical behavior. The metal-hydrogen systems have mean-field critical dynamics. To describe the hydrogen diffusion, a quantum mechanical model is constructed, based on cluster formation. The diffusion is regarded as a collective movement of clusters. The sizes of these clusters depend on interatomic forces and particle statistics. The observed reversed isotope effect is explained by different degrees of cluster formation in hydrogen and deuterium. The diffusion constants are calculated by solving the generalized Langevin equation via the method of recurrence relations.

Separations and Analysis, continued

KENT STATE UNIVERSITY
Kent, Ohio 44242

368. ADSORPTION AND DESORPTION OF HYDROCARBONS AT LOW CONCENTRATIONS — $56,500 — 02-02
Richard Madey
Department of Physics

The aim of this research is to study the adsorption and diffusion of hydrocarbon gases through porous media adsorber beds. The approach involves calculations based on a mass-balance equation of the quantity of adsorbate adsorbed on an adsorbent, measurements of adsorption isotherms of hydrocarbons on activated carbon and polystyrene beads at selected temperatures, and studies of the dynamics of breakthrough curves with both a step-function and a pulse change of the input concentration. The breakthrough curves of binary mixtures exhibit interference phenomena where the output concentration of the weakly-adsorbed component increases above the input concentration until the other component elutes. An objective of this study is to provide a quantitative explanation of interference phenomena. The approach will be to obtain binary adsorption isotherms, to examine the mechanisms of intraparticle diffusion and longitudinal diffusion of the system, and to study the mathematical characteristics of the differential equation that governs the system.

UNIVERSITY OF MINNESOTA
St. Paul, Minnesota 55108

369. INTERFACIAL CHEMISTRY IN SOLVENT EXTRACTION SYSTEMS — $80,000 — 02-02
Ronald D. Neuman
Department of Forest Products

This research project primarily aims at elucidating the interfacial behavior of extractant molecules and their interactions with metal ions using laser light-scattering techniques with a view to obtaining mechanistic insight into solvent extraction processes. Systematic investigations continue to examine the effect of pH of the aqueous phase, HDEHP concentration, and Ca^{2+} concentration on the interfacial properties of n-hexane/HDEHP/aqueous systems. The interfacial tension exhibits unusual behavior with increasing pH and suggests the presence of molecular aggregates. The fine structure of interfacial films is being examined by electron microscopy. Mass transfer studies on the extraction of Ca^{2+} from acidic aqueous solutions to n-hexane phase by HDEHP are being emphasized. Efforts are also being directed towards the study of spontaneous interfacial turbulence using Schlieren optical techniques. Attention is focusing on correlating interfacial properties with mass transfer rates and coalescence rates.

CALSPAN ADVANCED TECHNOLOGY CENTER
P.O. Box 400, Buffalo, New York 14225

370. ENERGY TRANSFER AND REACTION KINETICS OF VIBRATIONALLY PUMPED MOLECULES — $49,000 — 02-02
J. William Rich
Physical Sciences Department

This is a program of experimental and analytical research into energy transfer and reaction kinetics of vibration-to-vibration (V-V) pumped molecules. Extreme V-V pumped vibrational population distributions in CO, NO and other gaseous species are produced by optical excitation. Special emphasis is being placed on isotopic enrichment reactions of V-V pumped CO, which yield products enriched in ^{13}C, ^{17}O, and ^{18}O. Processes limiting vibrational up-pumping in CO and NO are being studied, especially vibration-to-electronic energy transfer from the pumped ground electronic state of these molecules to low lying excited electronic states.

Separations and Analysis, continued

UNIVERSITY OF GEORGIA
Athens, Georgia, 30602

371. FUNDAMENTAL STUDIES OF SEPARATION PROCESSES — $ 77,445 — 02-02
L. B. Rogers
Department of Chemistry

There are three major areas of effort in this research. The first is concerned with the fundamental aspects of two different forms of liquid chromatography, adsorption and steric exclusion, especially with respect to interaction during a given separation. Non-porphyrin compounds of vanadium and nickel and commercial mixtures of oligomers of polystyrene are ideal solutes for these studies because each type of sample covers a wide range of molecular weights. A second area involves the identification of those non-porphyrin compounds using a variety of techniques. The third area is concerned with recycle chromatography, a promising approach to separations of isotopic species.

TEXAS A&M UNIVERSITY
College Station, Texas 77843

372. INVESTIGATIONS ON MULTIPHOTON IONIZATION AND FAST-BEAM PHOTODISSOCIATION SPECTROSCOPY — $135,000 24 mo. FY 82-83 — 02-02
David H. Russell
Department of Chemistry

The emphasis of this research program is the development of combined laser-mass spectrometry methods for probing the dynamics of dissociation reactions. The experimental hardware and techniques are being developed using model chemical systems which have been characterized by other experimental methods, e.g., $C_6H_6^+$, $C_4H_6^+$, $C_4H_4^+$, etc. Following these preliminary investigations, the experimental capabilities will be applied to chemical systems which this approach provides unique or unusual capabilities. These latter studies emphasize the structural characterization of large molecular systems (1,000-10,000 a.m.u.). These large molecules are ionized using fast-neutrals (8-10 KeV Xe) and fast-ions (8-10 KeV Cs^+), i.e., fast-atom bombardment (FAB) and secondary ion mass spectrometry (SIMS), directly from the solid state. Also, these latter studies will be performed using a high resolution tandem mass spectrometer (Kratos MS-50TA) with high mass range capabilities (3,000-5,000 a.m.u.) and a Fourier transform mass spectrometer (Nicolet FTMS-2,000).

NATIONAL BUREAU OF STANDARDS
Washington, D.C. 20234

373. COMPETITIVE ION KINETICS IN DIRECT MASS SPECTROMETRIC ORGANIC SPECIATION — $125,000 — 02-02
L. Wayne Sieck
Center for Chemical Physics

This research involves the measurement of fundamental properties of gas phase ions, including fragmentation and reaction mechanisms and rates, structures, and the thermochemistry associated with ionization, protonation, and reaction. This information is then used to suggest chemical ionization techniques which incorporate competitive ion kinetics and permit identification and/or assay of specific compounds or classes of compounds occurring in complex organic mixtures. The experimental program utilizes the NBS pulsed high pressure mass spectrometer system as the prime facility, and an ion cyclotron resonance instrument is also available. Work-in-progress includes determinations of enthalpies of protonation, hydration, and solvation of complex amines, ethers, and sulfur compounds, as well as systematic studies of the unimolecular kinetics associated with ion pyrolysis.

Separations and Analysis, continued

SYRACUSE UNIVERSITY
Syracuse, New York 13210

374. MECHANISMS OF GAS PERMEATION THROUGH POLYMER MEMBRANES — $67,000 — 02-02
S. A. Stern
Department of Chemical Engineering and Materials Science

The objective of this study is to obtain a basic understanding of the mechanisms of gas permeation through nonporous polymer membranes. A "free-volume" model of gas permeation was found to describe satisfactorily the transport of many gases and of a number of gas mixtures through polyethylene membranes. The model is applicable at temperatures above T_g, the glass transition of the polymer, over a wide range of pressures. The validity of the model is being tested with other polymer membranes. Simple correlations of free-volume parameters have been developed. These correlations permit the prediction of diffusion and permeability coefficients for many gases and components of gas mixtures; solubility data are also required for this purpose. The gas permeation model has been extended to glassy polymers by incorporating in it the "dual-sorption" behavior observed below T_g. The extended model is being examined by means of "time-lag" and absorption-desorption measurements with a number of gases in poly(n-butyl methacrylate) over a temperature range encompassing T_g.

SYRACUSE UNIVERSITY
Syracuse, New York 13210

375. SELECTIVE METAL ION EXTRACTION FOR MULTIPLE ION LIQUID-LIQUID EXCHANGE REACTIONS — $82,000 — 02-02
Lawrence L. Tavlarides
Department of Chemical Engineering and Materials Science

This research in hydrometallurgical solvent extraction is to develop a fundamental means to predict selectivity during simultaneous solvent extraction of multiple metal ions when kinetic rates and thermodynamic equilibria do not favor the desired metal. The chemical kinetics and thermodynamic equilibria models for the system copper-iron-acid sulfate solutions extracted by β-alkenyl-8-hydroxy quinoline-xylene system are being determined. Iron extraction data have been obtained and analyzed to obtain a chemical equilibrium model. Kinetic experiments for the forward rate of the iron extraction are completed employing the liquid jet recycle reactor. Various models based on interfacial reaction mechanisms are under consideration. A one liter flow reactor system was designed, erected, and commissioned to acquire conversion and selectivity data. The system contains a photomicrographic assembly for drop size measurements, in situ membrane filtration for phase separation, and all wetted surfaces are inert to the process fluids. Simulation programs for predicting the extractor performance are on file to test the veracity of kinetic and extractor design models.

SYRACUSE UNIVERSITY
Syracuse, New York 13210

376. PARTICLE DEPOSITION IN GRANULAR MEDIA — $92,000 — 02-02
Chi Tien
Department of Chemical Engineering and Materials Science

This research is intended to obtain fundamental understanding of various phenomena arising from the flow of aerosol suspensions through and the deposition of aerosols in granular media. The study is focused on the following areas: (1) Experimental study of the transient state behavior of aerosol filtration in experimental filters; (2) The study of aerosol collection in magnetically stabilized fluidized filters and its modelling; and (3) The application of a specially designed two dimensional filter for in-situ observation of the change of media structure due to the retention of aerosol particles.

Separations and Analysis, continued

UNIVERSITY OF HOUSTON/Houston, Texas 77004
MARTIN-MARIETTA LABS/Baltimore, Maryland 21227

377. MECHANISMS OF CAKE FILTRATION — $164,108 — 02-02
Frank M. Tiller
Chemical Engineering-Univ. of Houston
Maher Tadros
Martin-Marietta Laboratories

This project is aimed at developing the theory of particulate separation involving compressible, porous beds or sediments as found in filtration, centrifugation, and sedimentation. A key feature of the investigation involves close collaboration between the University of Houston and Martin-Marietta Laboratories. Generation of reliable data and integration of the areas of pretreatment, thickening, and separation are objectives of the research. A rough predictive method for calculating parameters involved in functions relating porosity and permeability to effective pressure has been developed. Quantities used in the correlations include, particle size and shape and degree of aggregation. An apparatus for simulating a continuous thickener by partially fluidizing a bed of fine particles has been developed. Initial cake structure of deposits as affected by surface charge, suspension concentration, and agitation is being studied in relation to resistance to flow. Pressure distributions are used to study flow mechanisms and fine particle migration. The theory of centrifugal filtration of compressible cakes has been developed.

COLUMBIA UNIVERSITY
New York, New York 10027

378. UTILIZATION OF MAGNETIC EFFECTS AS A MEANS OF ISOTOPE ENRICHMENT — $62,000 — 02-02
Nicholas J. Turro
Department of Chemistry

This research program is directed toward the development of novel methods for the separation of isotopes based on exploitation of differences in magnetic properties of isotopes. Emphasis has been placed on discovering reactions and conditions which allow the separation of isotopes which possess a finite magnetic moment from those which do not possess a magnetic moment. Successful systems have been designed for separation of ^{13}C (a magnetic isotope) from ^{12}C (a non-magnetic isotope) and for the separation of ^{17}O (a magnetic isotope) from ^{16}O and ^{18}O (non-magnetic isotopes). The restricted space provided by porous silica has proven to be an excellent environment for efficient separation of ^{13}C and ^{12}C based on the photolysis of dibenzyl ketone. It should now be possible to design a practical system to separate these isotopes.

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, California 92717

379. STUDIES OF ISOTOPIC MASS EFFECTS IN CHEMISTRY — $75,000 — 02-02
Max Wolfsberg
Department of Chemistry

This project deals with theoretical studies of isotopic mass effects on molecular properties. Such work is usually carried out within the framework of the Born-Oppenheimer approximation. Exact expressions for the complete quantum mechanical Hamiltonian operator of molecules are being constructed to study this approximation. Statistical mechanical calculations of isotope effects on a variety of molecular properties require a knowledge of rotational-vibrational energies of molecules and of isotope effects on these energies. Such energies are being calculated by the variational method for formaldehyde, hydrogen cyanide and other molecules. The tunnelling phenomenon and isotope effects on tunnelling are being studied by an investigation of the vibrational energy levels of molecules with double-minimum potentials. Molecular dynamics calculations are being carried out on solutions of rare gases in water to elucidate isotope effects on Henry's law constants. The difference between gas phase and condensed phase infra-red spectra is being studied in connection with isotope effects on vapor pressures.

Separations and Analysis, continued

THE AEROSPACE CORPORATION
Los Angeles, California 90009

380. ISOTOPICALLY SELECTIVE, TWO-STEP, LASER PHOTODISSOCIATION OF MOLECULES — $107,597 — 02-02

P. F. Zittel
Chemistry and Physics Laboratory

This research program is directed toward understanding those photophysical, energy transfer, and chemical processes relevant to isotope separation by two-step laser photodissociation of small molecules. The two-step technique involves the vibrational excitation of molecules containing a chosen atomic isotope with an infrared laser, followed by ultraviolet laser photodissociation and scavenging of the photofragments. A computer-interfaced, dual beam, IR absorption apparatus is used to measure the absorption of intense IR laser pulses as a function of pressure and laser fluence. Mass spectrometric analysis of the photoproducts of the subsequent UV photodissociation step reveals the effect of vibrational excitation on the photodissociation cross section and gives the isotope enrichments. Of particular interest are measurements of vibrationally state specific photodissociation cross sections for different vibrational modes. Two-step photodissociation of OCS has led to the separation of all stable isotopes of O, C and S, to a determination of the dependence of the 249 nm photodissociation cross section on the amount of ν_2(bending) vibrational excitation, and to a rate constant for the exchange of bending vibrational energy between different isotopic varieties of OCS.

Chemical Engineering Sciences

STANFORD UNIVERSITY
Stanford, California 94305

381. TRANSPORT CHARACTERISTICS OF SLURRIES IN PIPELINES: FLOW REGIMES AND PRESSURE DROP — No Fund Extension — 02-04

Andreas Acrivos
Department of Chemical Engineering

This research aims to study the flow of slurries in pipelines from a fundamental point of view. Primary emphasis is placed on developing methods, based on sound scientific principles, for predicting the pressure drop and for delineating the various flow regimes that can occur in such systems. The theoretical framework is based on the equations of continuum mechanics and is being developed in close conjunction with a parallel experimental study. A theoretical model is currently being developed whose purpose is to explain quantitatively the curious and surprising phenomenon whereby a settled suspension was observed to resuspend in the presence of a laminar shear flow even under conditions of very small Reynolds numbers. It is believed that this resuspension is due to the action of a shear induced diffusion of particles, and attempts are currently being made to measure the corresponding diffusion coefficient. The possible connection between this shear induced diffusion and the measured normal stresses in the suspension is being investigated.

Chemical Energy Science, continued

COLUMBIA UNIVERSITY
New York, New York 10027

382. INTERACTION OF TURBULENCE and CHEMICAL REACTIONS — $85,000 — 02-04
Rene Chevray
Department of Mechanical Engineering

Flow in a two-dimensional mixing layer is utilized to study a well known reaction with simple kinetic scheme. The flow represents a well-defined turbulent situation and additional complexities of finite heat release are avoided by use of small concentrations for the reaction chosen ($NO + O_3 \rightarrow NO_2^* + O_2 \rightarrow NO_2 + h\nu + O_2$). Large Reynolds numbers, small dilution numbers, large reaction speed numbers and several concentration ratios are investigated. Conditional and conventional measurements are made of mean and fluctuating quantities for both the velocity and concentration fields by laser Doppler anemometry and absorption sprectroscopy, respectively. Simultaneous cinefilm recording is conducted in order to determine the convection velocity of the interface and hence the entrainment. Numerical simulation is set up to model directly the equations describing the evolution of the species concentrations in the shear layer.

THE JOHNS HOPKINS UNIVERSITY
Baltimore, Maryland 21218

383. PREDICTION OF THERMODYNAMIC PROPERTIES FOR COAL DERIVATIVES — $81,000 — 02-04
Marc D. Donohue
Department of Chemical Engineering

The purpose of this project is to develop an equation of state to predict the thermodynamic properties of coal derivatives. The equation is based on perturbed-hard-chain theory but includes additional terms for multi-pole interactions. The equation allows prediction of vapor pressures, densities, and solubilities for a wide range of organic molecules including multiringed aromatics. Pure component and mixture parameters are determined from experimental data when available; a group-contribution correlation is being developed to allow prediction of parameters for systems where no experimental data are available. The applicability of the new equation to supercritical fluid extraction is being studied. Hydrogen bonding effects are being taken into account to predict properties of systems containing H_2O, alcohol, etc. High pressure vapor-liquid equilibrium measurements for CO_2- aromatic binary mixtures are being made.

Chemical Engineering Sciences, continued

UNIVERSITY OF CALIFORNIA/DAVIS
Davis, California 95616

384. STATISTICAL MODELING AND ANALYSIS OF CHEMICALLY REACTING TURBULENT FLOWS
H. A. Dwyer
W. Kollmann

$145,000
24 mo.
FY 82-83

02-04

The research program is aimed at developing new turbulent closure models for variable density turbulent flows and turbulent diffusion flames. The techniques used to accomplish this goal are physical and mathematical modeling and sensitivity analysis. The physical and mathematical modeling studies have focused on density-velocity correlations in flows with pressure gradients and conditional statistics for modeling boundary intermittency. Also, the existing models have been applied to new experimental measurements with good results. The other effort of sensitivity analysis has been applied to both the compressible and incompressible round jet for the k-ε model. It has been shown that the conservation properties of the turbulent jet dominate the turbulence modeling, and that the turbulent jet has similar sensitivities to all turbulent model coefficients.

NATIONAL BUREAU OF STANDARDS/BOULDER
Boulder, Colorado 80303

385. EXPERIMENTAL AND THEORETICAL STUDY OF THE THERMOPHYSICAL PROPERTIES OF FLUID MIXTURES
Howard J. M. Hanley
Division 773

$195,000

02-04

The program is a coordinated task of experiment, theory, and correlation to study the properties and behavior of fluids. Specific objectives are: to produce PVT and thermodynamic data on hydrocarbon fluids and their mixtures at high temperatures (to 900 K) and pressures (to 35 MPa, possibly to 100 MPa); to develop the theory of liquids; and to develop models to predict the properties based on the theory and optimized by the data. A high temperature high pressure PVT apparatus has been completed and the PVT properties of H_2S to 520 K are available. The temperature range is being extended. A VLE/LLE phase equilibria apparatus is undergoing testing: preliminary results will be forthcoming for water/alcohol systems. Phase equilibria VLE measurements of the system CO_2/1-butane have been completed. Theoretical studies include computer simulation of fluids under shear. Studies are underway to investigate shear induced melting.

STANFORD UNIVERSITY
Stanford, CA 94305

386. FUNDAMENTAL STUDIES OF HEAT TRANSPORT, FLUID MECHANICS, AND STABILITY IN POROUS MEDIA
George M. Homsy
Department of Chemical Engineering

$84,789

02-04

This program treats problems in flow and transport phenomena in porous media whose solutions are of interest in energy recovery processes. Broad categories of activities include macroscopic and microscopic descriptions. Regarding former, theoretical and experimental studies of the effect of graded mobility on instabilities of displacement fronts have continued. The theory is being extended to study important effects of flow-induced dispersion and adsorption loss of the mobility control agent. Preliminary experiments in a Hele-Shaw cell have been completed, showing the stabilization of displacements due to mobility gradation. A theory of finite - amplitude thermally driven instabilities in bounded porous regions has been completed which determines the form of convection which will be observed. Microscopic studies of two phase Hele-Shaw flows have been completed with good agreement between theory and experiment. Microscopic modelling of non-Newtonian flow in porous media has been studied, indicating that constitutive equations of the Oldroyd type are incapable of capturing the salient experimental features of these flows.

Chemical Energy Science, continued

BRIGHAM YOUNG UNIVERSITY
Provo, Utah 84602

387. THERMODYNAMIC STUDY OF CO_2-ORGANIC COMPOUND INTERACTION AT HIGH PRESSURES AND TEMPERATURES. — $129,982, 24 mo., FY82-83 — 02-04

Reed M. Izatt, Department of Chemistry,
James J. Christensen, Department of Chemical Engineering

This research program is designed to gain increased understanding of the energetics associated with chemical interactions involving supercritical fluids. Emphasis is placed on reactions involving CO_2, Freons, and hydrocarbons. The quantities measured include heats of mixing of binary systems and heat capacities of individual components and mixtures. Flow calorimeters capable of operating to 673 K and 15 MPa are used to obtain the necessary experimental data. The variation of each measured quantity over the temperature and pressure ranges studied is described using equations involving existing theory and further theoretical development in our laboratory with particular emphasis given to critical point regions of the interacting fluid components.

THE CITY COLLEGE, C. U. N. Y.
New York, New York 10031

388. TURBULENCE AND THE DISTORTION OF REACTIONS — $50,000 — 02-04

Joseph A. Johnson III
Department of Physics

Contact surfaces in a pressure-driven shock tube are used as a way of investigating the possibility of the manipulation of molecular recombinations. Turbulent bursts are produced. The reaction $2NO_2+X \rightarrow N_2O_4+X$ (X=N_2 or Ar) is unstable under some circumstances; fluctuations with amplitude incoherence and phase coherence are developed. Here, the use of standard reaction rate data proves to be inadequate. The histories of flow and mixture properties are determined using cross-beam correlations and fluorescence of NO_2 probed by the 4.88 nm line from an Ar^+ ion laser. The importance of the dynamical parameters of of turbulence is being measured, specifically, the impact of changing local viscosity, characteristic turbulence scale, and turbulence intensity. In addition, there is some speculation that reduced molecular chaos may te relevant to this kind of process. This possibility is given a quantitative formulation and tested in our data.

NATIONAL BUREAU OF STANDARDS
Washington, D. C. 20234

389. TRANSPORT AND PHASE EQUILIBRIA IN MULTICOMPONENT FLUIDS — $70,000 — 02-04

John M. Kincaid
Thermophysics Division

The purpose of this project is to develop and implement simple, accurate techniques to treat the transport and phase transition properties of multicomponent systems. There are three basic aspects to the project: (1) the development of new techniques to study multicomponent systems; (2) the "translation" and adaptation of recent theoretical advances in transport and phase transition phenomena to forms usable to the energy technologies; (3) approximation assessment and implementation. All three of these areas can be expected to advance our understanding of multicomponent fluids at high temperatures. Recent progress includes: the development of a kinetic perturbation theory (1); the solution of several phase equilibria problems for polydisperse fluids (1); and molecular dynamics studies of diffusion in binary hard-sphere mixtures are being used to calibrate the Revised Enskog Theory (3).

STATE UNIVERSITY OF NEW YORK/STONY BROOK
Stony Brook, New York 11794

390. TRANSPORT PROPERTIES OF MULTIPHASE SYSTEMS — $165,000, 24 mo., FY 83-84 — 02-04
George Stell
Department of Mechanical Engineering

Ongoing research continues on the microscopic theory relating transport and structure in two-phase composite media, including new results on expected surface area and on quantitative comparisons of bounds and approximations that involve two-particle and three-particle correlations in such media. Research also continues on new statistical mechanical theories of transport at both liquid-state and gaseous-state densities. The liquid-state work includes the use of an entropy-maximization technique that leads to new quantitatively useful approximations for transport coefficients in the liquid state. The gaseous-state work includes the development of analytically tractable kinetic perturbation theories for useful model potentials. Finally, a kinetic approach to the theory of mixtures of interacting n-mers has yielded new exact results in the description of the gelation point and the post-gelation period for models that include and go beyond that of the Flory-Stockmayer theory.

CORNELL UNIVERSITY
Ithaca, New York 14853

391. EXPERIMENTAL AND THEORETICAL STUDIES OF DENSE FLUID MIXTURES — $180,000, 24 mo., FY 82-83 — 02-04
W.B. Streett and K.E. Gubbins
School of Chemical Engineering

The two principal goals of this research are: (1) carry out wide-ranging equation of state (PVT) measurements for pure fluids and mixtures; and (2) to develop improved methods for correlating, extrapolating and predicting dense fluid properties using statistical mechenics and intermolecular potential theory. Experimental research in progress includes measurements of the PVT properties of CF_4 from 120 to 230 K and pressures to 1000 bars. The direct-weighing PVT apparatus, designed and built under this project, has been completely redesigned and reconstructed to extend the temperature and pressure ranges to 0-600 C and 0-2000 bars, respectively. Theoretical work has included development of statistical mechanical methods for calculating properties of fluid mixtures containing hydrogen, at pressures up to 1000 bars. These methods are tested against experimental phase equilibrium and PVT data measured by our group.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

392. DYNAMICS OF VAPOR EXPLOSIONS — $46,050 — 02-04
B. Sturtevant
Graduate Aeronautical Laboratories

An experimental program to study an interfacial instability driven by rapid evaporation is continuing. The mechanism for the instability, which was discovered in previous experiments under this grant examining the vapor explosion of liquid butane heated to its superheat limit, is similar to that of the Landau instability of laminar flames. The previous experiments showed that the instability can cause the effective rate of vaporization of a single droplet of butane to be orders of magnitude greater than would be predicted by conventional theories of evaporating spherical bubbles. Recent calculations using an ad hoc Landau model have shown that the instability may be very sensitive to the ambient pressure, suggesting a method for controlling its effects. Presently, experiments are underway in a new apparatus that can be pressurized, in order to study the dependence of the vapor explosion of droplets of pentane on ambient pressure. Preliminary measurements of blast pressures indicate that the explosion is indeed qualitatively different at elevated pressures than it is at atmospheric pressure.

Basic Energy Sciences outlay funds are divided among operating, equipment and construction fudns. Equipment funds are provided primarily to DOE laboratories. (Operating funds provided to other contractors are used for all costs, including purchase of necessary equipment.) Chemical Sciences FY 1983 Equipment Funds were assigned as follows.

	Equipment Funds (K$)
Ames Laboratory	335
Argonne National Laboratory	885
Bartlesville Energy Technology Center	12
Brookhaven National Laboratory	1,383
Idaho National Engineering Laboratory	12
Lawrence Berkeley Laboratory	918
Lawrence Livermore National Laboratory	13
Los Alamos National Laboratory	52
Mound Facility	71
Notre Dame Radiation Laboratory	193
Oak Ridge National Laboratory	562
Pacific Northwest Laboratory	90
Pittsburgh Energy Technology Center	6
Sandia National Laboratories/Albuquerque	29
Sandia National Laboratories/Livermore	905
Solar Energy Research Institute	44

SPECIAL FACILITIES

The special facilities described on the following thirteen pages are supported wholly, or in part, by the Division of Chemical Sciences. They represent an assembly of unique and/or expensive equipment which would be costly to develop elsewhere. They represent research resources for the general scientific community and qualified scientists from laboratories outside the host laboratory are encouraged to make use of them. However, any activity which can be carried out through commercially available laboratories is not appropriate for these DOE supported facilities.

The process by which an off-site scientist can utilize a facility is discussed in each facility summary under the section "User Mode" for the National Synchrotron Light Source and the Combustion Research Facility or "Collaborative Use" for the remaining facilities. With the latter, the process is based on the need for collaboration by the off-site scientist with one or more in-house staff members.

Each of the facility summaries also gives the names of individuals to contact for further information, a general description of the facility and a list of technical data on the primary available instrumentation.

There are other facilities supported by the Office of Basic Energy Sciences (BES) which are not summarized here. Information concerning these can be obtained by contacting Dr. Louis C. Ianniello, Director of Materials Sciences, ER-13, U. S. Department of Energy, Washington, D.C. 20545.

Chemistry Division
Argonne National Laboratory
Argonne, Illinois 60439

ATOMIC SPECTROSCOPY FACILITY

The Argonne spectroscopic facility is designed for high-resolution investigations of atomic and molecular optical spectra, using a unique combination of large-scale dispersive instruments with state-of-the-art holographic gratings and pulsed, sharply-tunable coherent light sources for excitation energies of up to 11 eV. Photographic, Reticon array and resonance-ionization detectors, with associated data-processing equipment are available for a wide variety of experiments. Peripheral equipment includes a 50 KG superconducting magnet with a 24-inch room-temperature bore, high-temperature furnances for metal-vapor absorption tubes and an automatic plate-measuring comparator. YAG-laser-driven dye lasers are used with doublers and H_2-Raman scattering to cover the 2500-8500A range and to produce coherent radiation between 1180 and 1250 Å by four-wave mixing in mercury vapor at photon fluxes ranging from 10^{10} to 10^{16}/sec. for resolving powers of several million. The experimental work is reinforced by extensive computational programs for interpreting line broadening, diamagnetic, and hyperfine structure data in terms of fundamental atomic theories.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists.

PERSON TO CONTACT FOR INFORMATION

Henry M. Crosswhite
Chemistry Division (312) 972-3637
Argonne National Laboratory FTS 972-3737
9700 South Cass Avenue
Argonne, Illinois 60439

TECHNICAL DATA

Resolving power

30-foot Paschen-Runge spectrograph	$>5 \times 10^5$
5-meter Czerny-Turner spectrograph	$>10^6$
Tunable dye lasers	$>10^6$
Vacuum-ultraviolet coherent source	$>10^7$

Wavelength range, Å

30-foot Paschen-Runge spectrograph	2000-9000
5-meter Czerny-Turner spectrograph	1200-9000
Tunable dye lasers	2500-8500
Vacuum-ultraviolet coherent source	1180-1250

149

Physics Division
Argonne National Laboratory
Argonne, Illinois 60439

4.5-MV DYNAMITRON ACCELERATOR

The ANL Physics Division operates a high-current 4.5-MV Dynamitron accelerator which delivers magnetically analyzed beams of most atomic ions and many molecular ions. Among the facilities associated with the Dynamitron are (1) a beam line capable of providing "supercollimated" ion beams that permit angular measurements to accuracies of 0.1 mrad, (2) a beam-foil spectroscopy set-up with associated high-resolution photon (optical and X-ray) spectrometers, (3) a 28-inch diameter general-purpose scattering chamber, (4) a simultaneous irradiation system by which ion beams from the Dynamitron and from a 2-MV Van de Graaff accelerator are focussed onto the same target, (5) a variety of electron spectrometers including a high-resolution, large solid-angle McPherson spherical analyzer, and (6) a post-acceleration chopper system giving beam pulses with widths that can be varied from 1 nsec to several msec, at repetition rates variable up to 8 MHz. A PDP-11/45 computer system with a direct link to Argonne's central computing facility is used for on-line data acquisition, analysis and the control of experiments.

COLLABORATIVE USE

Visiting scientists use the accelerator either in collaboration with ANL investigators or as independent groups.

PERSON TO CONTACT FOR INFORMATION

D. S. Gemmell
Physics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

(312) 972-4053
FTS 972-4004

TECHNICAL DATA

Range of terminal voltages attainable	0.3 - 4.5 MV
Range of ion beam currents attainable	0.1 nA - 100 A
Monatomic singly-charged ion beams available	most elements
Monatomic multiply-charged ion beams available	rare gases, transition metals
Typical molecular-ion beams available	H_2^+, H_3^+, HeH^+, CH_n^+ (n=1,4), OH_n^+ (n=1,3), CO^+, O_2^+, etc.
Pulse mode (post-chopper)	
Pulse width	1 nsec - 10 msec
Repetition rate	1 MHz - 8 MHz

Chemistry Division
Argonne National Laboratory
Argonne, Illinois 60439

PREMIUM COAL SAMPLE PROGRAM

The purpose of the Premium Coal Sample Program is to provide the coal science research community with long term supplies of a small number of premium coal samples that can be used as standards for comparison. The premium coal samples produced from each coal and distributed through this program will be chemically and physically as identical as possible, have well characterized chemical and physical properties, and will be stable over long periods of time. Coals will be mined, transported, processed into the desired particle and sample sizes, and packaged in environments as free of oxygen as possible while maintaining the natural moisture content in order to insure that the coals will be in as pristine and stable a condition as possible.

AVAILABILITY

Initial samples are expected to be available in early 1984. Samples will be made available to research personnel at a nominal replacement cost. A very limited quantity of lump coal, stored under similar inert conditions will be available on special request for special physical property measurements. Distribution of these samples will be guided by policies established with the help of a users advisory committee. The processing facility may be available for occasional processing of special samples.

PERSON TO CONTACT FOR INFORMATION

Dr. Karl S. Vorres
Chemistry Division, Bldg. 200
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Phone: (312) 972-7374
FTS: 972-7374
Telex: TWX 910-258-3285 USDOE-CH ARGN

151

Chemistry Division
Argonne National Laboratory
Argonne, Illinois 60439

PULSE RADIOLYSIS FACILITY

The Argonne linear electron accelerator was designed for chemical research. The moderate energy of the electron accelerator (21 MeV transient mode, 14 MeV steady state) allows the use of the electron beam for the generation of transient species without nuclear activation. The pulse width can be varied from 25 picoseconds to 10 microseconds. In liquids, transient concentrations up to 20 micromolar may be generated with the 25 picosecond pulse and concentrations in excess of 10 millimolar may be generated with the longest pulse. Instrumentation for measurement of chemical processes allows kinetic spectrophotometric absorption and emission and fast conductivity measurements. Simultaneous multiwavelength kinetic spectrophotometric measurements are possible and very high time resolution measurements which utilize the short pulse capability of the linac can also be made both in absorption and emission. Other detection techniques such as resonance Raman spectroscopy are under development. All data acquisition equipment is computer interfaced to provide accurate data reduction. Sample preparation and handling facilities are available for solid, liquid and gaseous samples.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists.

PERSON TO CONTACT FOR INFORMATION

Charles D. Jonah
Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

(312) 972-3471
FTS 972-3471

TECHNICAL DATA

Energy	
Transient Mode	21 MeV
Steady State Mode	14 MeV
Pulse Repetition Rate	Single pulse - 800 pps (800 pps not possible for all pulses)
Current/pulse	
Transient Mode	20 amps
Steady State Mode	1.5 amps
Picosecond Pulse	25 nanocoulombs/pulse
Pulse Width	30 ps 4 - 100 ns .25 - 10 microseconds

162

National Synchrotron Light Source
Brookhaven National Laboratory
Upton, N.Y. 11973

NATIONAL SYNCHROTRON LIGHT SOURCE

The National Synchrotron Light Source (NSLS) facility consists of a 750 MeV (9 electron bunch) storage ring for VUV and IR research and a 2.5 GeV (30 electron bunch) storage ring for X-ray research. Attractive features of the synchrotron radiation include high brightness and intensity, its broad and continuous spectral range, high polarization and pulsed time structure (subnanosecond pulses). With each of the 28 X-ray and 16 VUV beam ports being further split into from 2 to 4 beam lines, it will be possible to have as many as 100 experiments running simultaneously at the NSLS. A 6 pole superconducting wiggler magnet and a 38 pole permanent magnet undulator have been constructed, and several wiggler and undulator magnets are presently being designed which will significantly increase the photon intensity and brightness.

The NSLS is a facility where a wide range of research techniques will be utilized by biologists, chemists, solid state physicists, metallurgists, and engineers for basic and applied studies. Among the techniques are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

USER MODE

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines are being designed and instrumented by "Participating Research Teams" (PRTs). The PRTs are given priority for up to 75% of their beam line(s) operational time for a three-year term.

General Users will be able to perform experiments on an NSLS facility beam line or on a PRT beam line which will be available for use by non-PRT members for at least 25% of its total operational time. In the latter case, PRTs will provide liaison and utilization support to General Users. After an initial commissioning period, NSLS and PRT beam lines will become available for use by General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee will be charged for the amount of beam time utilized. The DOE has granted the NSLS a Class Waiver, under the terms of which Proprietary Users of the NSLS will have the option to retain title to inventions that result from research performed at the Light Source.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky
NSLS - Bldg. 510E
Brookhaven National Laboratory
Upton, New York 11973

(516) 282-4974
(FTS) 666-4974

163

National Synchrotron Light Source, BNL, continued

TECHNICAL DATA

Facilities	Key Features	Operating Characteristics
VUV electron storage ring	high brightness, continuous wavelength range ($\lambda > 5$ Å) 16 beam ports.	0.75 GeV electron energy
X-ray electron storage ring	high brightness, continuous wavelength range ($\lambda > .5$ Å) 28 beam ports	2.5 GeV electron energy
Instruments		
Monochromators:		
plane grating	12 Å $< \lambda <$ 1500 Å; high resolution	
zone plate	8 Å $< \lambda <$ 100 Å; moderate resolution	
toroidal grating	10 Å $< \lambda <$ 2500 Å; high intensity, moderate and high resolution	
extended range grasshopper	20Å $< \lambda <$ 2000Å; high resolution	
Wadsworth	300 Å $< \lambda <$ 3000 Å; high intensity, moderate resolution	
Seya & Czerny Turner	1200 Å $< \lambda <$ 12000 Å; high intensity, moderate resolution	
two crystal	.04 Å $< \lambda <$ 2500 Å; high resolution, fixed exit beam	
two crystal/two grating	2.5 Å $< \lambda <$ 2500 Å; high resolution, fixed exit beam	
Six circle spectrometer/ diffractometers	high positional and rotational accuracy	
Experimental stations	photoemission, magnetic circular dichroism, fluourescence, gas phase spectroscopy, microscopy, lithography, holography, EXAFS, inelastic scattering, crystallography, radiometry, topography, small angle scattering	
Superconducting wiggler	$\lambda > .1$ Å; high intensity	
Permanent magnet undulator	100 Å $< \lambda <$ 1000 Å; high intensity and brightness	

154

Department of Physics
Kansas State University
Manhattan, Kansas 66506

JAMES R. MCDONALD LABORATORY

Three accelerators are operated primarily for atomic physics research. These accelerators are: a 6MV EN-tandem accelerator, a 3 MV Van de Graaff, and a 100 kV accelerator. Either foil or gas post-stripping between the 90° and switching magnet is possible for tandem beams. Available experimental facilities include: a) a 4.5 meter flight tube for impact parameter measurements, b) curve crystal x-ray spectrometer, c) spherical sector and cylindrical electron spectrometers, d) hydrogen atom and metal vapor oven targets, e) low-energy high-charge recoil ion sources, and f) Si(Li), proportional counter, avalanche, and channel-plate detectors. The laboratory is available to users who require the unique facilities of the laboratory for experiments pertinent to DOE program goals.

COLLABORATIVE USE

Users are encouraged to seek a collaborator on the staff or can submit a brief proposal.

PERSONS TO CONTACT FOR INFORMATION

Patrick Richard, Principal Investigator (913) 532-6783
or James C. Legg, Director (913) 532-6786
James R. Macdonald Laboratory
Department of Physics
Kansas State University
Manhattan, Kansas 66506

TECHNICAL DATA

EN tandem:

Beams: Most Elements

Terminal Voltages: 0.3 - 6 MV

Output Currents: Up to 10 μA depending on the ion species and charge state

Repetition Rate: DC or 3 nsec pulses at rates up to 4 MHz

Magnet Limitations: $ME/q^2 \lesssim 150$

J. R. Macdonald Laboratory, KSU, continued

3 MV Van de Graaff:

Beams: ^{1}H or ^{4}He

Terminal Voltages: 0.3 - 3 MV

Output Currents: Up to 100 μA

Repetition Rate: DC only

Magnet Limitations: None

100 kV Accelerator:

Beams: Most elements

Terminal Voltages: 20 - 100 KV

Output Currents: Up to 10 μA depending on the ion species

Magnet Limitations: None

158

Notre Dame Radiation Laboratory
University of Notre Dame
Notre Dame, Indiana 46556

PULSE RADIOLYSIS FACILITY

The Notre Dame pulse radiolysis facility is based on a 5 ns electron pulse from a 8 MeV linear accelerator. It is fully instrumented for computerized acquisition of optical and conductivity information on radiation chemical intermediates having lifetimes of 10 ns and longer. Detectors having response times of ~2 ns are available. For typical optical absorption studies, where one produces 10^{-5} M of intermediates, spectral and kinetic information can be obtained on species having extinction coefficients in excess of 100 $M^{-1} cm^{-1}$. Conductometric methods in aqueous solution cover the pH range of 3 to 11. Data are recorded digitally and stored in magnetically readable form for rapid off line examination of spectral and kinetic details.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists or by a proposal to the laboratory director.

PERSON TO CONTACT FOR INFORMATION

R. H. Schuler, Director (219) 239-7502
Notre Dame Radiation Laboratory FTS 333-8222
Notre Dame, Indiana 46556

TECHNICAL DATA

Electron source	8 MeV linear accelerator
Operating mode	single pulse, with signal averaging
Data collection	PDP 8
Pulse width	5, 10, 20, 50 ns
Time resolution (RC)	2 ns
Pulse current	up to 1 A
Repetition frequency	0.2 s^{-1}
Optical absorption Measurements	
Spectral region	210-750 nm
Sensitivity	$\pm$0.00002 absorbance
Conductivity	
pH range	3-11
Sensitivity	$\pm$5 mhos/cm

157

Notre Dame Radiation Laboratory
University of Notre Dame
Notre Dame, Indiana 46556

RADIOLYSIS-ESR FACILITY

The Notre Dame Radiolysis-ESR Facility is a unique facility for carrying out electron spin resonance studies directly in the microwave cavity during continuous or pulse electron radiolysis. The electron source is a 3 MeV Van de Graaff capable of irradiating continuously with currents up to 10 μA or in pulsed mode up to 1 A. The recording of spectra during irradiation allows species with lifetimes in the microsecond or longer range to be examined by steady state methods. Most radicals in solution have well resolved narrow lines so that hyperfine constants can be measured to ±0.02 G and g-factors to ±0.00002. The reaction kinetics of many small radicals can be followed directly by time resolved methods. This facilitiy is used for both quantative identification of radiation produced intermediates and for measurement of their electronic and kinetic properties.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists or by a research proposal to the laboratory director.

PERSON TO CONTACT FOR INFORMATION

R. H. Schuler, Director
Notre Dame Radiation Laboratory
Notre Dame, Indiana 46556

(219) 239-7502
FTS 333-8222

TECHNICAL DATA

Electron source	3 MeV Van de Graaff
ESR spectrometer	X BAND
Operating mode	Computer controlled field scan
Current - cw	10 μA
pulsed	0.1 A
Pulse width	0.1 μs to d.c.
Repetition rate	up to 100 kHz
Duty cycle	as needed
Field/frequency measurement	±0.02 G

Physics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

EN-TANDEM

The EN-Tandem is operated primarily as an atomic physics facility. The highest terminal voltage is 6.5 MV. The widest possible variety of ion species are available from a selection of ion sources. Two 90° magnets with a stripper (gas or foil) between them follow the accelerator so that a range of charge states is available for any ion at a given energy. Available facilities include: a) A merged-electron-heavy ion beam apparatus with a merged region $\sim$ 1 meter in length; b) a $\sim$ 14 meter flight tube with the capability of doing very small angle scattering and detecting individual charge states; c) a Penning ion trap apparatus; d) an Elbeck magnetic spectrograph with position sensitive detectors; e) Si(Li) detectors and a curved crystal spectrometer; f) both low- (eV to keV) and high- (MeV) monoenergetic position sources are being developed.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists or by a research proposal to the EN-Tandem manager.

PERSON TO CONTACT FOR INFORMATION

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Oak Ridge, TN 37830

(615) 574-4781
FTS 624-4781

TECHNICAL DATA

Beams: Most elements

Terminal Voltages: 0.3 - 6.5 MV

Source Beam Currents: Several hundred nA to several μA

Output Currents: Up to 1μA depending on the ion species, and charge state

Repetition Rate: DC only, at present

Magnet Limitations: $ME/q^2 \leq 80$

Combustion Sciences Directorate
Sandia National Laboratories/Livermore
Livermore, California 94550

COMBUSTION RESEARCH FACILITY

Current activities at the Combustion Research Facility (CRF) supported by the Division of Chemical Sciences emphasize both the development and applications of new diagnostic techniques to the study of basic flame processes, as well as research in fundamental chemistry important in combustion. (These programs are individually described elsewhere in this Summary Book). In addition, DOE/Conservation sponsors programs at the CRF in combustion technologies, and DOE/Fossil supports programs in coal combustion and related diagnostics development.

Complete facilities for resident and visiting researchers are available: offices for 60 staff, a meeting room accommodating 250 people, a laboratory building housing 14 independent experiments, special facility laser systems, a dedicated VAX computer, and access to a Cray computer.

The facility is located in the San Fransicso Bay area, near major universities and other U.S. Government-supported laboratories.

USER MODE

Qualified scientists are encouraged to take advantage of the specialized resources available at CRF. Prospective participants should submit a brief proposal to the laboratory director. Criteria for selection include technical merit, the extent to which CRF facilities are utilized, overlap with DOE program objectives, and the availability of specific equipment.

In general, the CRF will host visiting scientists to use the special-purpose lasers, work with resident staff, make use of computers and codes, and to set up experiments. Visitors pay for their own salary, travel, housing, meals, and other local expenses. Facility lasers, apparatus, technicians, instrumentation, computers, and the services of support groups are provided at no cost for research which is not proprietary. Research results from non-proprietary projects are expected to be published and disseminated.

For scientists with active government contracts, support for CRF research often can be arranged on an informal basis with the contract manager. There are opportunities for faculty, post-doctoral scientists, and graduate students to obtain Sandia support for combustion-related research at CRF.

Combustion Sciences Directorate, Sandia/L, continued
Combustion Research Facility

In specific instances, proprietary research can be carried out at CRF. For this type of work, the DOE will be reimbursed on a full cost recovery basis for the use of all CRF resources. Details of a DOE Class Waiver for patent rights are available.

PERSON TO CONTACT FOR INFORMATION

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--or--

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Combustion Sciences Department
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TECHNICAL DATA

Equipment	Key Features
Flashlamp-pumped, tunable dye laser	Long pulse, high energy, high average power: 2 microsecond pulse length; 5 Joules per pulse, 10 Hz; Tunable 440 to 620 nm; 0.03 nm bandwidth
Multi-purpose pulsed laser system	High peak power, high resolution doubled YAG and tunable dye lasers: Single mode capability; 10-500 mJ per pulse; 10-20 nanosecond pulse
Low pressure flames	10 microns to 1 atm. Mass spectrometer sampling probe
Atmospheric flames	Diffusion and premixed flames

161

Combustion Sciences Directorate, Sandia/L, continued
Combustion Research Facility

High pressure flame	Combination of diffusion flame burner with high pressure flow chamber: Pressures up to 20 atm.; Slot-geometry burner; 2-D laminar diffusion
Vertical turbulent diffusion flame	Open-circuit, induced draft wind tunnel with co-flowing axisymmetric fuel jet: 30 x 180 cm viewing section to 6000 scfm flow
Atmospheric Combustion Exhaust Simulator (ACES)	Atmospheric pressure combustion exhaust chamber: to 1200 degrees C; 0.5 - 100 m/s flow speed; Trace species and particulates; Optical and physical probes; Materials test section
Combustion bomb	Simulates constant-volume engine combustion
Internal combustion research engines	Highly repeatable environment for homogeneous charge and diesel combustion studies
Experimental diagnostics research facilities	Laser fluorescence laboratory
	Coherent Raman spectroscopy laboratories
	Laboratory for laser ionization, saturation, optogalvanic detection of trace species
	Kinetics laboratories with tunable quasi-cw uv and ring dye lasers for analysis; excimer lasers for photolysis
Computing facilities	Minicomputers in laboratories Access to CRF VAX 11/780 Access to SNLL CRAY via in-house staff

Topical Index

Analytical Spectroscopy
123, 126, 131, 133, 141, 142, 153, 156, 157, 351, 357, 358, 363, 364

Atmospheric Chemistry
4, 22, 52, 53, 100, 128, 165, 199, 257

Chromatography
124, 349, 366, 371

Combustion
4, 30, 38, 39, 42, 44, 49, 50, 52, 53, 55, 57, 58, 62, 63, 64, 65, 66, 67, 68, 158, 214, 217, 218, 220, 221, 222, 223, 224, 225, 226, 227, 228, 230, 231, 233, 234, 235, 236, 239, 240, 241, 242, 243, 245, 246, 247, 252, 253, 254, 256, 257, 258

Complexation for Separations
127, 134, 347, 352, 356, 360

Fluid, Particle Dynamics, and Transport Properties
87, 129, 160, 161, 162, 376, 377, 381, 382, 384, 385, 388, 389, 390, 391

Fossil Fuel Chemistry and Physics, including MHD
61, 84, 86, 90, 91, 101, 109, 114, 115, 116, 293, 295, 311, 313, 315, 332, 341, 387

Fusion
45, 70, 74, 75, 76, 77, 78, 79, 80, 136, 138, 265, 268, 270, 272, 273, 276, 277, 279, 282, 283, 287, 288

Heterogeneous Catalysis
23, 37, 43, 44, 47, 48, 51, 56, 58, 59, 60, 84, 85, 103, 105, 113, 118, 119, 174, 203, 213, 230, 232, 248, 255, 259, 296, 297, 298, 299, 300, 305, 306, 308, 310, 317, 319, 320, 322, 325, 326, 327, 328, 329, 331, 333, 334, 335, 336, 339, 342, 344, 345

Homogeneous Catalysis
82, 83, 88, 93, 99, 102, 103, 106, 120, 168, 292, 301, 302, 303, 304, 306, 307, 309, 312, 314, 316, 318, 323, 330, 333, 337, 338, 339, 340, 346

Hydrogen and Hydrides
47, 96, 107, 108, 110, 132, 136, 138, 146, 367

Isotope Effects and Separation
132, 136, 137, 138, 353, 354, 365, 367, 370, 378, 379, 380

Mass Spectroscopy
122, 125, 128, 135, 139, 140, 143, 154, 359, 362, 372, 373

Membrane Separations
121, 127, 350, 352, 355, 368, 374

Nuclear Fuel and Waste Processing
8, 145, 147, 150, 152

Radiation and Hot Atom Chemistry
4, 6, 8, 10, 13, 27, 28, 29, 31, 34, 163, 168, 172, 175, 177, 178, 183, 185, 186, 190, 192, 194, 196, 198, 200, 203, 211, 212

Resource Recovery
144

Solar Photo- and Bioconversion
2, 3, 5, 6, 7, 8, 9, 10, 11, 14, 15, 16, 17, 19, 20, 21, 23, 24, 26, 31, 32, 35, 36, 44, 84, 94, 97, 111, 117, 164, 166, 167, 169, 170, 171, 174, 176, 178, 179, 180, 181, 182, 185, 186, 188, 189, 191, 193, 194, 195, 197, 201, 202, 204, 205, 206, 207, 208, 209, 210, 213, 250

Solvent Extraction
121, 127, 145, 147, 149, 347, 360, 361, 369, 375

Thermodynamics
92, 95, 112, 159, 215, 321, 343, 383, 385, 387

Index of Offsite Institutions

Universities

University of Alabama
L. D. Kispert, 183

Amherst College
B. B. Benson, D. Krause, Jr., 353

University of Arizona
H. Freiser, 360
D. L. Lichtenberger, 248
G. Tollin, 206

University of Arkansas
M. Lieber, F. T. Chan, 279

Boston University
R. H. Clarke, 166
M. Z. Hoffman, 178
G. Jones II, 180

Brandeis University
H. Linschitz, 189

Brown University
G. J. Diebold, 357
E. F. Greene, 232
R. G. Lawler, 186

Brigham Young University
C. H. Bartholomew, 294
J. J. Christensen,
R. M. Izatt, 355, 387

California Institute of Technology
W. A. Goddard III, 230
R. H. Grubbs, 316
K. C. Janda, 238
A. Kuppermann, 184
B. Sturtevant, 392

University of California/Davis
H. A. Dwyer, W. Kollmann, 384
J. W. Root, 198

University of California/Irvine
W. J. Evans, 307
F. S. Rowland, 199
M. Wolfsberg, 379

University of California/Los Angeles
D. J. Cram, 356
M. A. El-Sayed, 169
M. F. Hawthorne, 318

University of California/Santa Barbara
P. C. Ford, 309
R. M. Martin, 251
R. G. Pearson, P. H. Barrett, 331
R. J. Watts, 209

University of California/San Diego
K. G. P. Sulzmann, 256

Carnegie-Mellon University
R. M. Richman, 197

University of Chicago
R. S. Berry, 215
W. J. Evans, 307
U. Fano, 267
J. C. Light, 249
L. M. Stock, 341

Clarkson College of Technology
J. H. Fendler, 171

Clemson University
J. D. Peterson, 195

University of Colorado
S. J. Cristol, 167
M. R. DuBois, 304
G. B. Ellison, 223
J. L. Falconer, 308
S. R. Leone, 246
S. J. Smith, 289

Universities (continued)

Colorado State University
C. M. Elliott, 306
J. K. Stille, 340

Columbia University
R. Bersohn, 216
R. Chevray, 382
G. W. Flynn, 173
N. J. Turro, 378

Cornell University
S. H. Bauer, 214
J. H. Freed, 310
V. O. Kostroun, 277
W. B. Streett, K. E. Gubbins, 391

Dartmouth College
C. L. Braun, 164

Drexel University
R. A. Mackay, 191

University of Florida
R. J. Hanrahan, 177

University of Georgia
T. G. Heil, 272
M. H. Lee, 367
L. B. Rogers, 371

Georgia Institute of Technology
A. R. Ravishankara, 253

Harvard Smithsonian Center for Astrophysics
A. Dalgarno, 266

University of Houston
L. Kevan, 182
F. M. Tiller, 377

Howard University
W. M. Jackson, 237

University of Illinois/Chicago Circle
R. J. Gordon, 231
J. H. Kiefer, 241
R. I. Walter, 208

Illinois Institute of Technology
J. M. Bowman, 217
D. Gutman, 234

Indiana University
M. H. Chisholm, 302
J. J. Gajewski, K. E. Gilbert, 311

Indiana-Purdue University/Indianapolis
P. W. Rabideau, 332

Jackson State University
J. Perkins, G. Miller, 285

Johns Hopkins University
M. D. Donohue, 383
W. S. Koski, 243

University of Kansas
G. M. Maggiora, 250
S.-I. Chu, 264

Kansas State University
T. W. Lester, J. F. Merklin,
C. M. Sorensen, 247
C.-D. Lin, 280
P. Richard, 287

Kent State University
R. Madey, 368

University of Kentucky
G. A. Sargent, E. B. Bradley, 336

Lehigh University
K. Klier, G. W. Simmons, 325

Louisiana State University
R. J. W. Henry, 273
N. R. Kestner, 181

Marquette University
S. L. Regen, 333

University of Maryland
D. L. Anderson, G. E. Gordon,
W. B. Walters, and W. H. Zoller, 348

University of Massachusetts
R. M. Barnes, 351

Universities (continued)

University of Massachusetts/Boston
H. van Willigen, 207

Massachusetts Institute of Technology
J. L. Kinsey, R. W. Field, 242
R. R. Schrock, 337
M. S. Wrighton, 213

University of Minnesota
R. Aris, R. W. Carr, Jr., 349
R. W. Carr, Jr., 165
W. E. Farneth, 225
W. R. Gentry, C. F. Giese, 229
S. Lipsky, 190
K. R. Maun, 330
K. D. Neuman, 369
D. G. Truhlar, 257

University of Missouri/Rolla
S. E. Friberg, P. Neogi, 361

University of Missouri/St. Louis
J. J. Leventhal, 278

Morehouse College
A. Z. Msezane, 282

Mt. Holyoke College
M. T. Spitler, 205

University of Nebraska
J. Macek, A. F. Starace, 281
G. G. Meisels, 192
E. P. Rack, 196
R. D. Rieke, 334

University of New Mexico
H. C. Bryant, 261

University of New Orleans
R. D. Kern, Jr., 240

City University of New York/City College
J. A. Johnson III, 388

New York University
B. Bederson, 260

State University of New York/Buffalo
H.-S. Kwok, 244

State University of New York/Stony Brook
J. Bigeleisen, 354
T. Ishida, 365
P. M. Johnson, 239
G. R. Stell, 390

Northwestern University
R. L. Burwell, Jr., T. J. Marks, 299
J. B. Butt, R. L. Burwell,
J. B. Cohen, 300
H. H. Kung, 326
D. F. Shriver, 339

University of North Carolina
T. Baer, S. A. Evans, Jr., 293
T. J. Meyer, 193
S. M. Shafroth, 288
D. G. Whitten, 210

Ohio State University
L. M. Dorfman, 168
R. F. Firestone, 172

University of Oklahoma
D. E. Golden, M. A. Morrison, 271

University of Oregon
P. C. Engelking, 224

Oregon Graduate Center
J. K. Hurst, 179

Pennsylvania State University
G. L. Geoffroy, 312
P. H. Given, 313
F. W. Lampe, 185
A. Sen, 338
M. A. Vannice, 342
P. L. Walker, Jr., R. G. Jenkins
F. J. Vastola, 322

University of Pittsburgh
P. Biloen, 296
D. M. Hercules, 320
J. T. Yates, 345

Princeton University
F. L. Dryer, 222
H. A. Rabitz, 252
T. G. Spiro, 204

University of Puerto Rico/Mayaguez
F. A. Souto, 202

Universities (continued)

Purdue University
G. Ascarelli, 163
R. A. Benkeser, 295
B. S. Freiser, 359
N. M. Laurendeau, D. W. Sweeney, 245

Rensselaer Polytechnic Institute
A. R. Cutler, 303
A. Fontijn, 228

Rice University
R. F. Curl, 221
R. E. Smalley, 255
G. K. Walters, N. F. Lane, 290

University of Rochester
J. M. Farrar, 226
W. D. Jones, 323
M. G. Raymer, 286

St. John Fisher College
F. T. Hioe, 274

San Diego State University
R. J. Laub, 366

Stanford University
A. Acrivos, 381
M. Boudart, 297
M. D. Fayer, 170
R. K. Hanson, 235
R. K. Hanson, C. T. Bowman, 236
G. M. Homsy, 386
R. J. Madix, 329

Syracuse University
S. A. Stern, 374
L. L. Tavlarides, 375
C. Tien, 376

Temple University
A. M. P. Goncalves, 176

University of Tennessee
S. D. Alexandratos, 347
D. J. Pegg, 284
T. F. Williams, 212

University of Texas
J. G. Ekerdt, 305
M. A. Fox, 174
J. W. Keto, 275

Texas A&M University
J. H. Fendler, 171
J. H. Lunsford, 327
M. P. Rosynek, 335
D. H. Russell, 372
R. L. Watson, 291

Texas Technological University
R. A. Bartsch, 352

University of Toledo
L. J. Curtis, 265

University of Utah
E. M. Eyring, 358
J. A. Gladysz, 314
D. M. Grant, R. J. Pugmire, 315
W. A. Guillory, 233
L. D. Spicer, 203

Vanderbilt University
C. F. Fischer, 268

University of Virginia
W. W. Harrison, 362

Washington University
P. P. Gaspar, 175

Wayne State University
A. Brenner, 298
D. M. Fradkin, 269
E. C. Lim, 188

Wesleyan University
A. R. Cutler, 303

The College of William and Mary
R. L. Champion, L. D. Doverspike, 263

University of Wisconsin
C. P. Casey, 301
F. F. Crim, 219
J. E. Willard, 211

Worcester Polytechnic Institute
A. A. Scala, 200

Wright State University
G. B. Skinner, 254

University of Wyoming
R. J. Hurtubise, 364

Universities (continued)

Yale University
R. D. Adams, 292
R. K. Chang, B. T. Chu,
M. B. Long, 218
G. L. Haller, 317
V. E. Henrich, 319
K. B. Wiberg, 343

Industrial and Other Laboratories

Aerochem Research Laboratories
W. Felder, 227

The Aerospace Corporation
J. A. Gelbwachs, 363
F. E. Hovis, 363
P. F. Zittel, 380

Bend Research Corporation
W. C. Babcock, 350

Calspan Advanced Technology Center
J. W. Rich, 370

Charles F. Kettering
Research Foundation
G. R. Seely, 201

Martin-Marietta Labs., Baltimore, Md.
M. Tadros, 377

National Bureau of Standards/Boulder
D. W. Norcross, 283
H. J. M. Hanley, 385

National Bureau of Standards/
Washington, D. C.
R. J. Celotta, D. T. Pierce, 262
J. M. Kincaid, 389
D. R. Lide, Jr., 187
T. E. Madey, R. D. Kelley, 328
P. Neta, S. G. Lias, M. Mautner, 194
L. W. Sieck, 373
W. Tsang, R. F. Hampson, 258

Owens-Illinois, Inc.
M. H. Keyes, 324

Rockwell International
S. J. Yosim, G. B. Dunks, 346

Smithsonian Astrophysical Observatory
J. L. Kohl, 276

Surface Analytic Research, Inc.
C. Y. Yang, 259

SRI International
D. R. Crosley, 220
T. F. Gallagher, 270
D. L. Hildenbrand, 321
H. Wise, J. G. McCarty, 344

INVESTIGATOR INDEX

Abell, G. C. 110
Acrivos, A. 381
Adams, R. D. 292
Alexandratos, S. D. 347
Anderson, D. L. 348
Andrews, M. A. 93
Angelici, R. J. 82
Appelman, E. H. 89
Areuni, P. 74
Aris, R. 349
Ascarelli, G. 163
Ashurst, W. T. 162
Babcock, W. C. 350
Baer, T. 293
Baes, C. F., Jr. 149
Baker, J. D. 134
Barnes, R. M. 351
Barr, P. 162
Barrett, P. H. 331
Barrows, R. D. 116
Bartholomew, C. H. 294
Bartlett, N. 98
Bartsch, R. A. 352
Basile, L. J. 89
Bauer, S. H. 214
Bautista, R. G. 121
Becker, R. L. 77
Bederson, B. 260
Bell, A. T. 105
Benjamin, B. M. 114
Benkeser, R. A. 295
Benson, B. B. 353
Benthusen, D. 65
Bergman, R. G. 99
Berkowitz, J. 69
Berry, H. G. 70
Berry, R. S. 215
Bersohn, R. 216
Beuhler, R. J. 45
Bielski, B. H. J. 10
Bigeleisen, J. 354
Biloen, P. 296
Blanch, H. W. 97
Bloomquist, C. A. A. 129
Bottcher, C. 77
Botto, R. E. 91
Boudart, M. 297
Bowman, C. T. 236
Bowman, J. M. 217
Bowman, M. G. 108
Bowman, M. 7
Bowman, R. C., Jr. 110
Bradley, E. B. 336
Braun, C. L. 164
Brenner, A. 298
Brown, L. L. 114
Brown, N. 50
Bryant, H. C. 261
Buchanan, A. C. III 115
Burger, L. L. 152
Burns, J. H. 149
Burwell, R. L., Jr. 299, 300
Busey, R. H. 112
Bushaw, B. A. 153
Butt, J. B. 300
Byers, C. H. 148, 161
Calvin, M. 19
Canon, R. M. 144
Carlson, T. A. 60
Carmichael, I. 33
Carr, R. 48
Carr, R. W., Jr. 165, 349
Casey, C. P. 301
Cattolica, R. 67
Celotta, R. J. 262
Chambers, R. R. 114
Champion, R. L. 263
Chan, F. T. 279
Chang, R. K. 218
Chen, M. J. 88
Cheng, K. T. 71
Cheng, R. K. 158
Chevray, R. 382
Childs, W. J. 72
Chipman, D. M. 24
Chisholm, M. H. 302
Christensen, J. J. 355, 387
Christie, W. H. 139,
Chu, B. T. 218
Chu, S. 264
Clark, J. H. 20
Clarke, R. H. 166
Clinton, S. D. 144, 146
Cohen, J. B. 300
Coleman, C. F. 145
Connick, R. E. 100
Connolly, J. S. 35
Conzemius, R. J. 122
Cooper, J. 36
Cram, D. J. 356
Crandall, D. H. 80
Crespi, H. L. 3
Creutz, C. 11
Crim, F. F. 219
Cristol, S. J. 167

Crosley, D. R. 220
Crosswhite, H. M. 41
Curl, R. F. 221
Curtis, C. J. 120
Curtis, L. J. 265
Cutler, A. R. 303
Dale, J. M. 141
Dalgarno, A. 266
Danesi, P. R. 127
Das, P. K. 25
Datz, S. 78
Davis, M. J. 42
Dekalb, E. 123
Delmore, J. E. 135
Diamond, H. 127
Dibble, R. 62
Diebold, G. J. 357
Dittner, P. F. 78
Donohue, D. L. 143
Donohue, M. D. 383
Dorfman, L. M. 168
Doverspike, L. D. 263
Dryer, F. L. 222
D'Silva, A. P. 123
DuBois, D. L. 120
DuBois, M. R. 304
Dunks, G. B. 346
Dunning. T. H., Jr. 42
Dworkin, A. S. 115
Dwyer, H. A. 384
Dyrkacz, G. R. 129
Eby, R. E. 139
Egan, J. J. 95
Eherenson, S. 44
Ekerdt, S. 305
Elliott, C. M. 306
Ellison, G. B. 223
El-Sayed, M. A. 169
Engelking, P. C. 224
Erpenbeck, J. J. 160
Espenson, J. H. 83
Evans, S. A., Jr. 293
Evans, W. J. 307
Eyring, E. M. 358
Fahlman, A. 60
Fajer, J. 14
Falconer, J. L. 308
Fano, U. 267
Farneth, W. E. 225
Farrar, J. M. 226
Farrow, R. 66, 68
Fassel, V. A. 123
Fayer, M. D. 170
Feldberg, S. 15
Felder, W. 227
Fendler, J. H. 171
Ferraudi, G. J. 26
Ferrieri, R. A. 13
Fessenden, R. W. 27, 28
Field, R. W. 242
Firestone, R. F. 172
Fischer, C. F. 268
Fisher, P. W. 146
Flesch, G. D. 40
Flower, W. 63
Flynn, G. W. 173
Fontijn, A. 228
Ford, P. C. 309
Fox, M. A. 174
Fradkin, D. M. 269
Frank, A. J. 36
Franz, J. A. 116
Freed, J. H. 310
Freiser, B. S. 359
Freiser, H. 360
Friberg, S. E. 361
Friedman, L. 45
Fritz, J. S. 124
Funabashi, K. 29
Gaffney, J. S. 131
Gajewski, J. J. 311
Gallagher, T. F. 270
Gammon, B. E. 92
Gaspar, P. P. 175
Gelbwachs, J. A. 363
Gemmell, D. S. 73
Gentry, W. R. 229
Geoffroy, G. L. 312
Gerstein, B. C. 84
Giese, C. F. 229
Gilbert, K. E. 311
Given, P. H. 313
Glasdysz, J. A. 314
Glish, G. L. 140
Goddard, W. A., III 230
Golden, D. E. 271
Goldsmith, J. 64
Goncalves, A. M. P. 176
Goodman, D. W. 119
Goodman, L. S. 72
Gordon, B. M. 133
Gordon, G. E. 348
Gordon, R. J. 231
Gordon, R. L. 154
Gordon, S. 8
Grant, D. M. 315
Greenbaum, E. 111
Greene, E. F. 232

Greene, J. P. 69
Grover, J. R. 46
Grubbs, R. H. 316
Gubbins, K. E. 391
Guillory, W. A. 233
Guse, M. P. 110
Gusinow, M. A. 63, 65, 66
Gutman, D. 234
Hagaman, E. W. 114
Haller, G. L. 317
Hampson, R. F. 258
Hanley, H. J. M. 385
Hanrahan, R. J. 177
Hanson, R. K. 235, 236
Harbottle, G. 130
Harding, L. B. 42
Hardwick, J. 30
Harris, C. B. 51
Harrison, W. W. 362
Hawthorne, M. F. 318
Hayatsu, R. 91
Heiberger, J. J. 88
Heil, T. G. 272
Heineman, H. 101
Helman, W. P. 33
Henrich, V. E. 319
Henry, R. J. W. 273
Hercules, D. M. 320
Hildenbrand, D. L. 321
Hill, F. B. 132
Hillman, M. 16
Hindman, J. C. 5
Hioe, F. T. 274
Hoffman, D. K. 37
Hoffman, M. Z. 178
Hohimer, J. P. 81, 157
Holmes, H. F. 112
Holroyd, R. A. 10
Homsy, G. M. 386
Horwitz, E. P. 127
Houk, R. S. 125
Hovis, F. E. 363
Hug, G. 33
Hulett, L. D. 141
Hurst, J. K. 179
Hurtubise, R. J. 364
Ishida, T. 365
Izatt, R. M. 355, 387
Jackson, W. M. 237
Janda, K. C. 238
Jarvinen, G. D. 109
Jenkins, R. G. 322
Jepson, B. E. 137
Jessup, J. S. 134
Johnsen, R. 65
Johnson, B. M. 75
Johnson, J. A., III 388
Johnson, P. M. 239
Johnston, H. S. 22
Johnston, S. 62, 63
Jolly, W. L. 102
Jonah, C. 4, 6, 8
Jones, G., II 180
Jones, K. W. 75, 133
Jones, W. 108
Jones, W. D. 323
Kalina, D. 127
Kanter, E. P. 73, 74
Kaplan, L. 127
Katz, J. J. 3, 5
Kaye, J. H. 153, 155, 156
Kee, R. 67
Kelley, J. M. 154
Kelley, R. D. 328
Kern, R. D., Jr. 240
Kestner, N. R. 181
Keto, J. W. 275
Kevan, L. 182
Keyes, M. H. 324
Kiefer, J. H. 241
Kincaid, J. M. 389
Kinsey, J. L. 242
Kispert, L. D. 183
Klemm, R. B. 49
Klier, K. 325
Klinger, R. J. 88
Kniseley,, R. N. 123
Koetzle, T. F. 47
Kohl, J. L. 276
Kollmann, W. 384
Koski, W. S. 243
Kostroun, V. O. 277
Koszykowski, M. 64
Kozak, J. J. 24
Kraner, H. W. 133
Krause, D., Jr. 353
Krause, M. O. 60
Kubas, G. J. 109
Kudo, H. 74
Kung, H. H. 326
Kuppermann, A. 184
Kvick, A. 47
Kwok, H.-S. 244
Lampe, F. W. 185
Landsman, S. D. 117
Lane, N. F. 290

Laub, R. J. 366
Laurendeau, N. M. 245
Lawler, R. G. 186
Layne, C. 66
Lee, M. H. 367
Lee, Y. T. 52, 59
Leone, S. R. 246
Lester, T. W. 247
Lester, W. A., Jr. 53
Leventhal, J. J. 278
Lias, S. G. 194
Lichtenberger, D. L. 248
Lide, D. R., Jr. 187
Lieber, M. 279
Light, J. C. 249
Lim, E. C. 188
Lin, C.-D. 280
Linschitz, H. 189
Lipsky, S. 190
Livingston, R. 61
Long, M. B. 218
Lu, K. T. 41
Lunsford, J. H. 327
Macek, J. 281
Mackay, R. A. 191
Madey, R. 368
Madey, T. E. 328
Madix, R. J. 329
Maggiora, G. M. 250
Mann, K. R. 330
Marks, T. J. 299
Marrus, R. 76
Marshall, W. L. 112
Martin, R. M. 251
Mason, G. W. 127
Mautner, M. 194
McBay, E. H. 140
McBeth, R. M. 91
McCarty, J. G. 344
McClelland, J. F. 123
McConville, G. T. 138, 149
McDowell, W. J. 145
McKown, H. S. 143
McLean, W. 63, 67
McMullan, R. K. 47
Meisel, D. 6, 8
Meisels, G. G. 192
Merklin, J. F. 247
Mesmer, R. E. 112
Meyer, T. J. 193
Michael, J. V. 49
Michaels, E. D. 137
Miller, G. 285
Miller, J. A. 67
Miller, J. R. 6
Miller, P. D. 78, 79
Miller, W. H. 54
Mitchell, R. 67
Moak, C. D. 78
Molton, P. M. 117
Moore, C. B. 55
Morgan, L. G. 152
Morrison, M. A. 271
Mozumder, A. 29
Msezane, A. Z. 282
Muckerman, J. T. 44
Muetterties, E. L. 103
Mulac, W. 4, 6
Nelson, D. A. 117
Neogi, P. 361
Neta, P. 31, 194
Netzel, T. L. 11
Neuman, R. D. 369
Newman, J. 104
Newton, M. D. 44
Ng, C. Y. 38
Norcross, D. W. 283
Norris, J. 3, 7, 9
Nozik, A. J. 36
Onstott, E. 108
Otvos, J. W. 19
Overbury, S. H. 113
Owyoung, A. 81, 157
Palmer, D. A. 112
Palmer, R. 68
Pandolphi, R. 69
Parkinson, B. A. 36
Parks, E. K. 43
Patterson, L. K. 32, 34
Pearson, R. G. 331
Pegg, D. J. 284
Perkins, J. 285
Perona, J. J. 161
Perry, R. 63
Petersen, J. D. 195
Pfeufer, V. 72
Phaneuf, R. A. 80
Pierce, D. T. 262
Pimental, G. C. 21
Pitzer K. S. 56
Poutsma, M. L. 113, 114
Prausnitz, J. M. 159
Premuzic, E. T. 131
Pruett, D. J. 144, 147
Pugmire, R. J. 315
Pulsifer, A. H. 87

Rabideau, P. W. 332
Rabitz, H. A. 252
Rack, E. P. 196
Rahn, L. 68
Ramsey, J. M. 142
Rathke, J. W. 88
Ravishankara, A. R. 253
Raymer, M. G. 286
Regen, S. L. 333
Reilly, J. J. 96
Rich, J. W. 370
Richard, P. 287
Richman, R. M. 197
Rickert, P. G. 127
Rieke, R. D. 334
Riley, S. J. 43, 158
Robben, F. 158
Robertson, D. M. 154
Rogers, L. B. 371
Root, J. W. 198
Ross, A. B. 33
Ross, H. H. 142
Rosseel, T. 141
Rosynek, M. P. 335
Rowland, F. S. 199
Ruedenberg, K. 39
Ruscic, B. 69
Russell, D. H. 372
Russell, J. A. 117
Rutherford, W. M. 137
Ryan, R. R. 109
Sanders, B. R. 162
Sargent, G. A. 336
Sauer, M. C. 8
Saykally, R. J. 57
Sayre, E. V. 130
Scala, A. A. 200
Schaefer, H. F. 58
Schefer, R. 62
Schmidt, K. H. 6, 8
Schmieder, R. 63
Schneider, D. 74
Schrader, G. L. 85
Schrock. R. R. 337
Schuler, R. H. 34
Schwarz, H. A. 10
Scott, R. G. 91
Seely, G. R. 201
Seltzer, S. 94
Sen, A. 338
Shafroth, S. M. 288
Sham, T. K. 48
Shaw, R. W. 142
Shepard, R. L. 42
Shirley, D. A. 59
Shriver, D. F. 339
Sieck, L. W. 373
Simmons, G. W. 325
Skinner, G. B. 254
Skotheim, T. 15
Small, G. J. 1
Smalley, R. E. 255
Smart, J. C. 120
Smith, A. V. 81, 157
Smith, D. H. 143
Smith, F. J. 150
Smith, G. P. 115
Smith, R. D. 151
Smith, S. J. 289
Smooke, M. 67
Somorjai, G. A. 23, 105
Sorensen, C. M. 247
Souto, F. A. 202
Spicer, L. D. 203
Spiro, T. G. 204
Spitler, M. T. 205
Starace, A. F. 281
Stein, L. 89
Stell, G. R. 390
Stencel, J. M. 118
Stern, S. A. 374
Stevens, C. M. 128
Steward, S. A. 107
Stille, J. K. 340
Stock, L. M. 341
Stoenner, R. W. 130
Stoffels, J. J. 154
Stoffler, W. 74
Streett, W. B. 391
Struve, W. S. 2
Sturtevant, B. 392
Styris, D. L. 156
Sulzmann, K. G. P. 256
Sutherland, J. W. 17
Sutin, N. 11
Svec, H. J. 40, 122
Sweeney, D. W. 245
Tadros, M. 377
Talbot, L. 158
Tavlarides, L. L. 375
Taylor, R. D. 136
Taylor, W. L. 138
Thurnauer, M. C. 6, 7
Tien, C. 376
Tiller, F. M. 377
Todd, P. J. 139, 140

Tollin, G. 206
Tomkins, F. S. 41
Toth, L. M. 147
Trahanovsky, W. S. 86
Trifunac, A. D. 8
Tripathi, G. N. R. 30, 34
Truhlar, D. G. 257
Tsang, W. 258
Tully, F. P. 64
Turner, J. A. 36
Turro, N. J. 378
Ulrichson, D. L. 87
Vannice, M. A. 342
van Willigen, H. 207
Vastola, F. J. 322
Vollhardt, K. P. 106
Vorres, K. S. 90
Wagner, A. F. 42
Walker, P. L., Jr. 322
Walker, R. L. 143
Walter, R. I. 208
Walters, G. K. 290
Walters, W. B. 348
Warner, R. A. 153
Wasielewski, M. R. 3, 7, 9
Watson, J. S. 148
Watson, R. L. 291
Watts, R. J. 209
Wells, G. F. 79
Weston, R. E. 12
Wexler, S. 43
Wham, R. M. 148
White, M. 46
Whitten, D. G. 210
Whitten, W. B. 142
Wiberg, K. B. 343
Wilke, C. R. 97
Wilkes, W. R. 137
Willard, J. E. 211
Williams, T. F. 212
Winans, R. E. 91, 129
Wise, H. 344
Wolf, A. P. 13
Wolfsberg, M. 379
Woodward, J. 111
Wrighton, M. S. 213
Yang, C. Y. 259
Yates, J. T., Jr. 345
Yeung, E. S. 126
York, R. W. 138
Yosim, S. J. 346
Young, J. P. 142
Zingg, S. P. 115
Zittel, P. F. 380
Zoller, W. H. 348

F. Nuclear Sciences Subprogram

1. What is the detailed budget structure of the Nuclear Sciences subprogram? What types of work are funded by each of these budget categories?

Answer: The detailed budget structure of the Nuclear Sciences Subprogram is Nuclear Data, Isotope Preparations and Heavy Element Chemistry, Stanford Synchrotron Radiation Laboratory, and Heavy Ion Fusion Accelerator Research.

The goal of the Nuclear Data Subprogram is to establish and maintain an accurate, complete, and accessible nuclear data base to meet long-term needs of the nuclear technologies; fission and fusion energy, and nuclear defense systems. The subprogram supports a system, which includes nuclear data measurements compilation, evaluations, and dissemination services. This includes the support of the Oak Ridge Electron Linear Accelerator, ORELA, and of the National Nuclear Data Center at BNL.

Isotope Preparations and Heavy Element Chemistry supports two efforts: (a) the service function of providing samples of enriched stable isotopes and of the actinide elements for DOE research programs, sales, and loans; and (b) the research into the basic chemical and physical properties of the heavy (actinide) elements.

Nuclear Sciences funding at SSRL is for the operation of the facility to provide high quality and steadily improving synchrotron radiation for much of the user community in the U.S. and the Free World. SSRL shares equally with the High Energy Physics program the operating time and costs of SPEAR (Stanford Positron - Electron Asymmetric Ring).

The Heavy Ion Fusion Accelerator Research program supports the development of heavy ion accelerator technology and associated ion-beam experiments to develop an adequate data base for evaluation of heavy ion inertial fusion drivers for their possible use in civilian power applications of inertial confinement fusion. For this purpose a six-year, two-stage program plan has been formulated starting in FY 1984.

2. For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.

Answer: The funding by year for the Nuclear Sciences Subprogram is:

	B/A (M $)				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating					
Nuclear Data	7.65	8.52	8.82	9.43	11.38
Isotope Preparations and Heavy Element Chemistry	12.04	13.08	15.95	16.93	22.10
Stanford Synchrotron Radiation Laboratory	0	0	5.89	6.79	7.98
Heavy Ion Fusion Accelerator	0	0	0	4.75	8.30
Subtotal Nuclear Sciences - Operating	19.69	21.60	30.66	37.90	49.76

	B/A (M $)				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Equipment					
Nuclear Data	0.33	0.35	0.36	0.38	0.70
Isotope Preparations and Heavy Element Chemistry	0.49	0.52	0.74	1.03	1.00
Stanford Synchrotron Radiation Laboratory	0	0	0.46	0.49	0.60
Heavy Ion Fusion Accelerator Research	0	0	0	0.25	0.65
Subtotal Nuclear Sciences - Equipment	0.82	0.87	1.56	2.15	2.95
Construction					
Nuclear Data	0	0	0	0	0
Isotope Preparations and Heavy Element Chemistry	0	0	0	0.27	0.30
Stanford Synchrotron Radiation Laboratory	0	0	0	0	0
Heavy Ion Fusion Accelerator Research	0	0	0	0	0
Subtotal Nuclear Sciences - Construction	0	0	0	0.27	0.30
Total Nuclear Sciences	20.51	22.47	32.22	40.32	53.01

3. **For the period FY 1981 - FY 1985, please identify, by budget category and by facility, that portion of Nuclear Sciences funding going for the support of facilities, such as the Oak Ridge Electron Linear Accelerator (ORELA), etc.**

Answer: The funding by year and budget category for Nuclear Sciences facilities is:

	B/A (M $)				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Operating					
Nuclear Data-ORELA	1.26	1.40	1.52	1.65	1.80
Isotope Preparations and Heavy Element Chemistry					
Calutrons	1.32	1.18	0.82	0.68	1.70
High Flux Isotope Reactor	4.28*	4.72*	5.59	6.15	7.82
Transuranium Processing Plant	3.68	4.10	4.90	5.14	5.49
Stanford Synchrotron Radiation Laboratory	0	0	5.89	6.79	7.98
Heavy Ion Fusion Accelerator Research	0	0	0	0	0
Total Nuclear Sciences	10.54	11.40	18.72	20.51	24.79

*Contains comparability for funding transferred from Materials Sciences: FY81 = $0.78M and FY82 = $0.92M

4. For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Nuclear Sciences funding going to DOE laboratories.

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
NUCLEAR SCIENCES
LABORATORIES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC01 NUCLEAR SCIENCES					
KC0101 NUCLEAR DATA					
OPERATING EXPENSES					
AMES LAB	$ 200	$ 185	$ 0	$ 0	$ 0
ARGONNE NATIONAL LAB	2220	2150	0	0	430
BROOKHAVEN NATIONAL LAB	4527	5323	1910	2057	2800
IDAHO NATIONAL ENG. LAB	265	320	290	300	520
LAWRENCE BERKELEY LAB	1510	1360	300	375	395
LAWRENCE LIVERMORE NAT LAB	470	437	220	210	220
LOS ALAMOS NATIONAL LAB	1055	1095	950	1005	1055
OAK RIDGE NATIONAL LAB	3482	3985	3212	3480	3840
PACIFIC NORTHWEST LABS	250	200	244	250	260
SANDIA CORP	6	0	0	0	0
KC0102 ISOTOPES PREPARATION AND HEAVY ELEMENT CHEMISTRY					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	835	1145	1237	1300	1390
LAWRENCE BERKELEY LAB	937	1085	1204	1230	1320
LAWRENCE LIVERMORE NAT LAB	0	0	45	0	0
LOS ALAMOS NATIONAL LAB	240	320	338	375	420
MOUND LABORATORY	111	149	157	140	232
OAK RIDGE NATIONAL LAB	8546	9770	12483	13191	17770
SANDIA CORP	19	0	0	0	0
KC0104 HEAVY ION FUSION RESEARCH					
OPERATING EXPENSES					
LAWRENCE BERKELEY LAB	0	0	0	3530	4400
LOS ALAMOS NATIONAL LAB	0	0	0	920	1600
STANFORD UNIVERSITY-SLAC	0	0	0	50	50

(B/A In thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
35KC01 NUCLEAR SCIENCE					
CAPITAL EQUIPMENT					
ARGONNE NATIONAL LAB	101	90	100	100	100
BROOKHAVEN NATIONAL LAB	32	40	40	50	50
IDAHO NATIONAL ENG LAB	25	25	25	25	25
LAWRENCE BERKELEY LAB	80	85	90	265	590
LAWRENCE LIVERMORE NAT LAB	5	0	0	0	0
LOS ALAMOS NATIONAL LAB	89	83	140	145	225
OAK RIDGE NATIONAL LAB	450	472	645	950	1240
PACIFIC NORTHWEST LABS	23	20	20	20	20
39KC00					
CONSTRUCTION					
OAK RIDGE NATIONAL LAB	0	0	0	270	300

5. **For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of Nuclear Sciences funding going to universities.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
NUCLEAR SCIENCES
UNIVERSITIES
(B/A In thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
KC0101 NUCLEAR DATA					
OPERATING EXPENSES					
CLARK UNIVERSITY	$ 58	$ 58	$ 0	$ 0	$ 0
COLORADO SCHOOL MINES	0	0	47	75	60
COLORADO UNIV OF	719	400	0	0	0
CORNELL UNIV	67	55	0	0	0
DENISON UNIVERSITY	28	34	49	49	40
DUKE UNIV	980	1265	0	0	0
FLORIDA STATE UNIV	0	3	0	0	0
GEORGIA INS OF TECHNOLOGY	43	43	0	0	0
INDIANA UNIV	- 1	0	0	0	0
IOWA STATE UNIV - AMES	110	0	0	0	0
KENTUCKY UNIV OF	60	0	0	0	0
LOWELL UNIV OF	92	116	120	124	130

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
MARYLAND UNIV OF	65	79	0	0	0
MASSACHUSETTS INST TECH	20	- 40	0	0	0
MICHIGAN UNIV OF	130	153	153	170	180
MIDDLE TENNESSEE STATE	35	32	0	36	40
NEW MEXICO UNIV OF	42	51	106	56	60
NEW YORK CITY U - BROOKLYN	142	153	0	0	0
NEW YORK ST UNIV OF ALBANY	38	39	41	0	0
NORTH CAROLINA STATE U	145	175	80	56	55
NORTH CAROLINA UNIV OF	170	191	0	0	0
NORTH TEXAS STATE UNIV	0	8	0	0	0
OHIO UNIV	150	195	215	235	250
OKLAHOMA UNIV OF	0	45	0	0	0
OREGON STATE UNIV	0	0	30	0	0
PENNSYLVANIA UNIV OF	89	89	96	92	95
TEXAS A & M UNIV	460	600	0	0	0
WASHINGTON UNIV OF	735	1339	0	0	0
WISCONSIN UNIV OF	723	514	0	0	0
YALE UNIV	500	659	0	0	0
KC0102 ISOTOPES PREPARATION AND HEAVY ELEMENT CHEMISTRY					
OPERATING EXPENSES					
FLORIDA STATE UNIV	77	82	89	96	102
MAINE UNIV OF	0	- 11	0	0	0
NEW MEXICO UNIV OF	0	64	74	73	78
STANFORD UNIVERSITY-SSRL	0	100	0	0	0
TENNESSEE TECH UNIV	0	66	0	0	0
TENNESSEE UNIV OF	202	219	224	235	268
KC0103 STANFORD SYNCHROTRON RADIATION LABORATORY					
OPERATING EXPENSES					
STANFORD UNIVERSITY-SSRL	0	0	5894	6736	7880
35KC01 NUCLEAR SCIENCES					
CAPITAL EQUIPMENT					
STANFORD UNIVERSITY-SSRL	0	0	456	490	600

6. **For the period FY 1981 - FY 1985, please provide, by budget category and by company, the amount of Nuclear Sciences funding going to industrial researchers.**

Answer: Please see the table for the requested information.

BASIC ENERGY SCIENCES
NUCLEAR SCIENCES
INDUSTRY
(B/A In thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC01 NUCLEAR SCIENCES					
KC0101 NUCLEAR DATA					
OPERATING EXPENSES					
ROCKWELL INTER. CORP.	$ 75	$ 100	$ 110	$ 120	$ 120
KC0102 ISOTOPE PREPARATION AND HEAVY ELEMENT CHEMISTRY					
OPERATING EXPENSES					
PRINTING - DOE R&D REPORT	- 7	0	0	0	0
35KC01 NUCLEAR SCIENCES					
CAPITAL EQUIPMENT					
ROCKWELL INTER. CORP.	0	20	15	10	0

7. **For the period FY 1981 - FY 1985, please provide, by budget number and by agency, the amount of Nuclear Sciences funding going to other agencies.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
NUCLEAR SCIENCES
FEDERAL
(B/A In thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NUCLEAR SCIENCES					
KC0101 NUCLEAR DATA OPERATING EXPENSES					
NAT BUREAU OF STANDARDS	$ 545	$ 580	$ 620	$ 630	$ 670
KC0104 HEAVY ION FUSION RESEARCH OPERATING EXPENSES					
NAVAL RESEARCH LAB	0	0	0	120	100
35KC01 CAPITAL EQUIPMENT					
NAT BUREAU OF STANDARDS	25	25	25	25	30

8. **How much of the FY 1985 Nuclear Sciences budget request is for support of programs formerly funded by the DOE Nuclear Program or by any other DOE program?**

Answer: For the Nuclear Data subprogram, $1.4M in FY 1985 operating expense funds is provided for a program formerly funded by DOE Nuclear Energy programs.

None of the Isotope Preparations and Heavy Element Chemistry budget is for programs formerly funded by other DOE programs.

The Stanford Synchrotron Radiation Laboratory funding is also a relatively recent addition to the Nuclear Sciences budget. This program was previously funded by the National Science Foundation and was transferred to DOE starting with the FY 1983 budget.

The Heavy Ion Fusion Accelerator Research program was transferred October 1, 1984 from the Defense Program Office of Inertial Fusion (DP/IF) to the Office of Energy Research. The program was restructured and redefined to emphasize evaluation of accelerator technology, with a small fusion target design subprogram remaining in the DP/IF program. Thus, it is considered a new program in the Nuclear Sciences budget, replacing a program formerly funded by DP/IF.

9. **What have been the major accomplishments of this subprogram over the past five years?**

Answer: Major accomplishments are described below which are typical of the research supported in this subprogram.

NUCLEAR DATA

New Measurement of California-252 Neutron Yield Standard

The spontaneous fission of californium-252 is used as a standard against which measurements of the interaction of neutrons with nuclei, from any source, including other fissioning isotopes (e.g., uranium-235 and plutonium-239), are made. A significant nuclear data effort has produced a new and definitive measurement of the average number of neutrons emitted per fission (a parameter called nubar) for californium-252. This experimental program, carried out over a period of five years, has resulted in an unprecedented accuracy for this type of measurement. The uncertainty assigned to the new value of nubar is less than 0.2%. Achieving this accuracy involved painstaking experiments and exhaustive analysis of possible experimental errors. This new measurement, besides its fundamental importance in neutron physics research, has immediate impact on fuel cycle costs in light water reactors. The fission fuel consumption rate in reactors depends strongly on the value of nubar and more cost effective scheduling of fuel cycles and fuel enrichment can be achieved if nubar is known to very high accuracy. It has been estimated that savings of $250,000 per fuel cycle per reactor can be realized solely on the basis of the improved accuracy resulting from this work. Economies in designing fast breeder reactors would also be realized. The californium-252 used in these experiments was produced at the High Flux Isotopes Reactor (HFIR) at Oak Ridge.

(Oak Ridge National Laboratory, R. Spencer, P. Gwin, and R. Ingle)

Detailed Measurement of Charged Particle Production by 14 MeV Neutrons Made Possible by Specially Designed Spectrometer System

Materials bombarded by fusion neutrons are altered by nuclear transformations which produce hydrogen and helium. To assess the potential performance of specific materials for fusion reactor applications, cross-section data are required by the fusion community and the Office of Fusion Energy.

The required cross-sections are difficult to measure because of the relative weakness of available fast neutron beams, the requirement for thin targets to permit the escape of the charged particles produced, and the large backgrounds associated with fast neutrons.

In order to make much better measurements of the energy spectra and angular distributions of the charged particles under these conditions, magnetic lens systems have been developed, first at LLNL and more recently at Ohio University, to capture, focus, and transport these charged particles from the reaction target to a remote well-shielded detector.

Measurements at the high particle energy of 14 MeV encountered in fusion reactions have been completed for the materials designated to be of interest to the Fusion program, e.g., Li, Be, B, C, N, O, F, Al, Si, Ti, V, Cr, Fe, Ni, Cu, Nb, Mo, Sn, W, and Pb. The measurements made for low mass number nuclides are also of interest to others, e.g., for neutron theory studies. The detector systems have now been improved to such an extent that it has become possible to measure cross-sections at fast neutron energies other than those in the 14-15 MeV range at the very intense LLNL Rotating Target Neutron Sources where this work was carried out. Measurements have been made at the Ohio University high current tandem Van de Graaff at 8 MeV for ^{58}Ni and 316-stainless steel.

(Lawrence Livermore National Laboratory, R. C. Haight; Ohio University, R. O. Lane)

Neutron Reaction Cross Sections by New Technique

High resolution measurements of neutron and gamma ray production cross sections have been made for the first time for neutron bombardment energies above 15 MeV. These measurements were made simultaneously over the range from 200 keV to 40 MeV using the intense pulsed beam time-of-flight system at the Oak Ridge Electron Linear Accelerator (ORELA) and were made possible by a new technique based on a high resolution lithium-doped germanium detector. Although these cross sections are of primary interest to the Office of Fusion Energy, the initial measurement provided information of timely importance to the fast reactor program, clearing up a troublesome discrepancy between experimental and theoretical results for an important design benchmark, the "large iron sphere". The measurement of the isotope iron-57 demonstrated that this minor component of natural iron (2.2% abundance) can not be ignored in the calculation. The observation of a surprisingly intense gamma-ray line, the measurement of which was made possible by the high resolution detector used, also has provided valuable information for the theorists who are developing a complicated nuclear model for the calculation of these cross sections.

The cross sections being measured with the new system are of interest not only for direct input into calculations of neutron transport and activation, but are also contributing to the development of a computational model that will permit the prediction of cross sections for high energy neutron reactions that are difficult or time-consuming to measure, but are needed for inclusion in the Evaluated Nuclear Data File (ENDF) maintained by DOE.

(Oak Ridge National Laboratory, D. Larson)

HEAVY ELEMENT CHEMISTRY

Plutonium Specific Complexing Agent Synthesized

A new class of chelating (from Greek for "claw") agents has been synthesized, one of which has been found to remove plutonium selectively from animal tissues. This class of chemical compounds has been designed on a molecular scale to satisfy two criteria crucial to precise selectivity: geometric configuration to fit that of the plutonium species to be removed, and a chemical bonding match to a plutonium ion bearing a plus four charge. The immediate interest has been in the application of the newly synthesized LICAM-C (linear catechoylamide carboxylate) to living systems where it was shown that, with minimal side effects, one dose of LICAM-C removed, through the kidneys, 70% of the plutonium injected into mice. This work has attracted attention in the public press, and LICAM-C has received publicity as a potential decontaminating agent in the case of accidents involving uptake of plutonium by people. Less dramatic, but of perhaps greater significance, is the possibility of tailoring chemical extractants to treat both nuclear and chemical wastes for removal of noxious species and recovery of valuable materials from dilute sources.

(Lawrence Berkeley Laboratory, K. Raymond, F. Weitl)

Fluorescence of Actinides: Highly Sensitive Monitoring Technique

Clever choices of laser excitation frequencies have enabled measurement of fluorescence spectra and lifetimes of actinides in aqueous solution. This may make possible routine monitoring of actinides in process chemistry and in the aquatic or geologic environment. Early studies of actinide emission spectra had indicated that the fluorescence spectrum and lifetime of curium species in the +3 valence state should be observable but not those of other +3 actinides. The curium (+3) fluorescence has now been measured in remarkably dilute concentrations of about 10^{-9} molar. Further detailed studies using carefully chosen laser excitation have now shown that similar observations are also possible for einsteinium (+3), and almost certainly for berkelium (+3) and americium (+3). These techniques are being extended to other valence states of the actinides so that similar information can be obtained for uranium, neptunium, and plutonium. Since the energy and lifetime of fluorescence radiation is highly sensitive to the identity of the actinide species and its valence state this information may lead to the development of powerful techniques for monitoring actinides.

(Argonne National Laboratory, J. Beitz)

Leaching of Plutonium from Glass Host Materials Into Water Increased by High Radiation Fields

One of the mechanisms responsible over long time periods for the transport of radioactive species from one location to another is leaching. The radioactive species or any species that is soluble, is dissolved or made mobile by local groundwater and transported to some other location where it precipitates or is deposited. The extent to which this mechanism affects radioisotope movement is important in dealing with long term nuclear waste isolation. Previous studies on the effects of high radiation conditions on the rate at which plutonium can be leached out of materials have dealt with only the solid glass system and water not exposed to radiation for any extensive periods. Recent studies were conducted on an expanded system consisting of the glass which contains actinide elements and an aqueous medium in a high radiation field. These studies have shown that the strong oxidizing and reducing reactants formed during the irradiation of the aqueous medium significantly increase the amount and rate of leaching of plutonium from a standard sample of a glass material. This aspect of the effect of radiation on a glass/aqueous system was not fully recognized heretofore. It has also been shown that a significant fraction of the leached plutonium is associated with colloidal silica particles which also result from the irradiation of the glass. This association could increase the mobility of plutonium from a breached repository. The results of this research provide additional insight important in the design of nuclear waste isolation systems.

(Argonne National Laboratory, J. C. Sullivan)

Clarified Picture of the Chemistry of Plutonium in Environmentally Important Aqueous Media

All bodies of water contain dissolved carbon dioxide which, on solution, forms either the carbonate or bicarbonate ion. These two species are in dynamic equilibrium with bicarbonate dominating in the more acidic solutions and carbonate in the more basic ones. This dynamic equilibrium tends to maintain the acidity level in the system and is called buffering. A comprehensive picture of the chemistry of plutonium species and certain other actinides in environmentally important aqueous carbonate-bicarbonate media has been developed.

Combination of electrochemical and spectroscopic techniques has produced the first comprehensive picture of the reduction-oxidation chemistry of plutonium and certain other actinides in carbonate-bicarbonate media. Many inland lakes and groundwaters are bicarbonate-buffered; and, this study has identified the environmentally important or stable oxidation states of plutonium in such media to be Pu(IV) and Pu(VI) and not Pu(V). Pu(V) has been found to be stable in the more alkaline, carbonate-buffered media found, for example, in limestone deposits. Natural reducing conditions such as iron deposits can lead to possible immobilization of the plutonium (IV), (V), or (VI) by the precipitation of Pu(III) products. Preliminary studies with uranium and neptunium show few chemical similarities with plutonium and indicate considerable complexities in actinide environmental chemistry. This new insight strongly contributes to our understanding of the behavior of actinides in the environment.

(Argonne National Laboratory, Dennis W. Wester)

Natural Soil Substances Shown Likely to Retard Migration of Plutonium and Other Actinides

Studies on the chemical binding of actinide elements to naturally occurring humic materials -- organic portions of soils -- indicate that migration of plutonium through soil rich in humic materials would be very slow. Naturally occurring humic materials are polymeric substances which are known to bind metal ions well and are found in soils and both fresh and marine waters. Data for absorption of americium, thorium, and uranium ions from aqueous solutions show that the complexing, and hence retention of these ions by the complex organic species in humic materials is strong and increases as the solution becomes more basic. Calculations of the competition for Pu(IV) - plutonium's most probable form - between hydrolysis in the aqueous solution at midrange pH values and binding to humic materials show that the binding is significantly competitive and sometimes dominant at normal environmental concentrations. Further studies of the dissociation of thorium (IV) humate show that a significant portion of the bound metal ion is essentially kinetically inert. Thus, to the extent that Th(IV) mimics the chemical behavior of Pu(IV), these results indicate a very slow migration of plutonium through soils rich in humic materials due both to the high binding constants and the very slow dissociation rate of most of the bound metal ions at low acidities. These and related studies suggest that there exists a variety of geomedia, humates as well as minerals, that adsorb and strongly bind actinides and would restrain their migration from a repository.

(Florida State University, Gregory R. Choppin)

First Detection of Fluorescence Emission from Electronically Excited Plutonium Hexafluoride Has Been Achieved

The first detection of fluorescence emission from electronically excited PuF_6 has been achieved. This directly impacts the development of methods for the laser-based separation of plutonium isotopes.

Fluorescence has been observed in an initial study of plutonium hexafluoride vapor using visible wavelength laser excitation. This is the first observation of fluorescence from electronically excited plutonium hexafluoride. The large differences in electronic energy levels and in molecular dissociation limits make it likely that plutonium hexafluoride will not mimic uranium hexafluoride. This has been confirmed in this scouting study of selective laser excited plutonium hexafluoride.

The small fluorescence quantum yield but long fluorescence lifetime suggest that a complex mixture of energy transfer and dissociation reactions simultaneously occur when plutonium hexafluoride absorbs visible wavelength light. Experimental tests of this interpretation are being undertaken and efforts are being made to identify the emitting state. This work directly impacts on efforts to separate plutonium isotopes by providing the first information concerning the dynamics of electronically excited plutonium hexafluoride.

(Argonne National Laboratory, J. V. Beitz)

First Measurement Made of Metallic Vapor Pressure of Einsteinium

The first measurement of the metallic vapor pressure of the man-made element number 99, einsteinium, has been made using material produced and prepared in the High Flux Isotope Reactor and Transuranium Processing Plant at the Oak Ridge National Laboratory. This is the heaviest and also highest atomic number element for which this fundamental thermodynamic measurement has been made. From the experimental data the investigators have derived a value of 31.2 kilocalories per gram-molecular weight for the energy required to vaporize the metal from a solid to a gas. This information is valuable for the increase in our understanding of the fundamental chemical and physical properties of elements and of their behavior in chemical reactions.

The measurements indicate that einsteinium is a divalent metal, like calcium and magnesium, and thus quite unlike the lighter actinide element metals. This confirms earlier predictions based on the observed trend in the higher actinides, of the increasing stability of the divalent as compared to the trivalent state.

Einsteinium may well be the last element in the Periodic Table for which this type of measurement can be made because the next higher element, fermium, can thus far only be produced in hundred-million-fold smaller quantities.

(Los Alamos National Laboratory, J. Ward, and Oak Ridge National Laboratory, R. Haire)

Stanford Synchrotron Radiation Laboratory

DOE's funding of the SSRL through the Nuclear Sciences subprogram enables it to be operated to serve users who carry out research supported almost entirely by other sources. Thus the flow of research accomplishments by SSRL staff and creditable to the Nuclear Sciences subprogram is limited. There are noteworthy advances, however, in the design and operation of improved sources of synchrotron radiation. Recently, for example, the world's most intense x-ray beams were produced by SSRL's new 54-pole wiggler (a sequence of magnets between which the synchrotron's electron beam passes).

Heavy Ion Fusion Accelerator Research

This is a newly transferred and reshaped activity.

10. **For the period FY 1981 - FY 1985, how much funding has this subprogram provided and is estimated to provide for the R&D of experiental devices/apparatus?**

Answer: Capital Equipment funding for the FY 1981-FY 1985 period is shown in the table included in the answer to Question 2 above. Additional small items of equipment are purchased with operating expenses funds. For Nuclear Data, the largest item for this period is the $0.4M replacement of the ORELA data acquisition computer included in the FY 1985 Presidential Budget.

For Isotope Preparations we have mounted a three-year campaign totalling $1.2M in FY's 83-85 to upgrade the coolant circulating and vacuum systems at the Calutron facility.

The costs of R&D for the design and fabrication of new experimental devices/apparatus cannot usually be determined with any reasonable degree of accuracy because such R&D is usually integral with the conduct of the basic research program.

11. **How does the research funded by the Nuclear Sciences subprogram differ, complement, supplement, or overlap nuclear science research funded by other parts of DOE, as well as by other agencies such as the National Science Foundation?**

Answer: The BES/Nuclear Data program has become the major supporter and backbone of the U.S. nuclear data system. Other DOE Offices, as well as the National Bureau of Standards and the Electric Power Research Institute (EPRI), contribute to the system by supporting some measurement efforts and some data evaluators. These contributions are coordinated by the National Nuclear Data Center (NNDC) through the Cross Section Evaluation Working Group (CSEWG) and are incorporated by the NNDC into the National Evaluated Nuclear Data File (ENDF).

The Heavy Element Chemistry research effort is focused on the study of the basic chemical and physical properties of the actinide elements. This is not specifically funded elsewhere in DOE. This basic research effort complements and supplements DOE nuclear energy research and development in nuclear fuel form and reprocessing, actinide waste host research, behavior of actinides in the environment, and the removal of actinides from biological systems. The related research funded by Nuclear Energy, Defense Programs, and Health and Environmental Research usually comprises shorter term efforts focused on specific practical problems. The researchers funded by Heavy Element Chemistry are frequently associated with those funded by the technology programs at the National Laboratories, so that cross-fertilization results. The National Science Foundation and the Department of Defense basic research programs have no research focused on the actinides, but some of their grants include some actinide research. Information to minimize undesirable overlap in the research programs is exchanged between the agencies in periodic meetings, telephone contacts, and project listings.

The Stanford Synchrotron Radiation Laboratory (SSRL), like the National Synchrotron Light Source (NSLS) funded at Brookhaven by Materials Sciences and Chemical Sciences, provides synchrotron radiation for advanced researchers in physics, chemistry, biology and medicine. Prominent at both is research on materials of many types and purposes. They complement each other in that SSRL currently provides several x-ray beams including the world's most intense synchrotron x-ray source, while the emphasis at NSLS is currently on ultraviolet radiation until its second ring becomes operational and provides x-ray beams intense enough for research use. The two facilities supplement each other in that the needs of all qualified researchers for synchrotron radiation beam lines cannot be met by existing facilities. Past projections of today's importance and demand for synchrotron radiation beam lines have been significantly exceeded.

The Heavy Ion Fusion Accelerator Research program is unique in terms of the primary goal: the development of very high current, heavy ion accelerators for inertial fusion application. Such accelerators differ from conventional accelerators for nuclear physics by many orders of magnitude in required

beam current. With this key qualification, the program leans heavily on, and is synergistic with, the decades of accelerator development sponsored by the DOE, the NSF, and the Department of Defense. The program complements the Inertial Fusion program supported in the Defense Programs (DP) budget in the sense that the DP program supports methods of inertial fusion of near term interest to defense applications, whereas the HIFAR program is supported solely on the basis of its energy production potential.

12. **What types of formal and informal advisory groups are employed to assure that the subprogram is of high quality and coordinated with the research carried out at other agencies? If any formal advisory groups exist, please define the role of each, and provide a listing of the current membership.**

Answer: An informal DOE Nuclear Data Peer Review Group consisting of a member from each of the National Laboratories involved in the nuclear data system, plus representatives from interested government offices, provides advice to the laboratory Nuclear Data program manager. A panel of the National Research Council/National Academy of Sciences provides advice on the part of the program involved in the compilation and evaluation of nuclear structure and decay data that is entered into the Evaluated Nuclear Structure Data File (ENSDF) from which the Nuclear Data Sheets, and other publications, are produced for use by the nuclear research and technology communities.

The Heavy Element Chemistry research Program at each lab is reviewed annually for quality and coordination by formal meetings between lab staff and DOE management. The National Research Council/National Academy of Sciences is occasionally called upon to review a specific area of research or address a specific question. Interagency coordination is effected by means of the Informal Federal Interagency Chemistry Representatives Group. Information exchanged at Group meetings includes budget data, program trends, and areas of emphasis and declining interest. These meetings thus help prevent unnecessary overlaps in program content and foster coordination in the handling of proposals sent to more than one agency.

The Stanford Synchrotron Radiation Laboratory receives advice from its Science Policy Board, a group of five Prominent scientists. The Board reports formally to the President of Stanford University. Members are H. Frauenfelder (University of Illinois), W. Brinkman (Bell Laboratories), D. Shirley (Lawrence Berkeley Laboratory), W. Phillips (Washington University) and H. Mark (NASA). A Proposal Review Panel reviews and assigns ratings to proposals or research at the SSRL experimental stations. There is also an SSRL Users Organization which advises SSRL on matters pertinent to user interests. Its members include scientists who are familiar with and often users of other synchrotron radiation facilities. In this framework for assuring high quality and coordination with other synchrotron radiation facilities, no duplicating group directly advisory to DOE on SSRL's Program has been needed.

No formal advisory group is used for regular evaluation of the Heavy Ion Fusion Accelerator Research Portion of the Nuclear Science subprogram. In 1983, however, a JASON committee reported on its evaluation of Heavy Ion Fusion research. The review was initiated in connection with the transfer of this accelerator research from Defense Programs to Energy Research. The JASON committee endorsed the program plan recently initiated in the Nuclear Sciences subprogram, calling it a "--minimal and sensible next step--."

13. Has the number of nuclear sciences researchers supported by this subprogram been increasing, stable, or decreasing over the past five years? What change will occur given the FY 1985 budget request?

Answer: The number of researchers in the nuclear data area has decreased slightly over the past five years, as the support from the fast breeder program has weakened. The FY 1985 President's Budget for the BES/Nuclear Data subprogram attempts to maintain that part of the data effort that can best be justified from the longer range perspective of the national nuclear data program.

The number of investigators in the Heavy Element Chemistry research effort has remained stable over the past five years. No appreciable change is anticipated given the FY 1985 budget request.

Most of the scientists whose proposals are on the active list of the Stanford Synchrotron Radiation Laboratory are researchers from other institutions, funded by various Federal agencies and private organizations. The numbers of these researchers has ranged from about 430 in 1979 to about 550 in 1983. No significant changes are seen at this time.

The number of researchers in the Heavy Ion Fusion Accelerator Research program is increasing as the program expands to the level required by the six-year, two-stage program plan to evaluate the heavy ion inertial fusion energy production method. However, much of the specific increase in FY 1985 will be used to fabricate components required for a series of multiple-beam experiments to validate the methods chosen for development.

14. What is the average annual cost per year to this subprogram to support a nuclear sciences researcher?

Answer: The average annual cost to support a researcher in the Nuclear Data and Heavy Element Chemistry programs is estimated to be $140,000. This estimate is derived by dividing total research funding by the total number of researchers supported on an annual basis by the program. At the Stanford Synchrotron Radiation Laboratory most of the researchers using the facility are visitors from other institutions and not supported by Nuclear Sciences. For the Heavy Ion Fusion Accelerator Research program this estimate is $170,000 which includes materials, component fabrication, computing, etc. and is computed in a similar manner as Heavy Element Chemistry.

15. Please provide a copy of the latest Nuclear Sciences research summaries.

Answer: Attached is a copy of the latest Nuclear Sciences summary book.

DOE/ER-0061
UC-2, 34e

Summaries of FY 1980 Research in the Nuclear Sciences

June 1980

U.S. Department of Energy
Directorate of Energy Research
Division of Nuclear Sciences
Washington, DC 20545

Dear Colleague:

For fiscal year 1978 the DOE Division of Nuclear Sciences issued a descriptive booklet entitled "Summaries of FY 1978 Research in the Nuclear Sciences." These summaries constitute the basic document by which the Nuclear Sciences Program of DOE's Office of Basic Energy Sciences can be made known in some technical detail to interested people. It is addressed to those in government and the scientific community who may wish to learn of the nature of the research being conducted under the support of this program.

For the FY 1980 edition we request that you and/or your colleagues provide for us by May 1, 1980, an up-to-date one-page summary of the Nuclear Sciences activities under your cognizance. Please retain the same format as the enclosed example but delete the AK-OW-OX-OY-Z budget and reporting classification, the fiscal year designation, and the funding level. To minimize the retyping burden and publishing delays, please provide finished copy ready for reproduction. The summaries should be complete and self-contained providing information on project scope and objectives and avoiding undue speculation about future plans. Please address your replies to S. L. Whetstone or J. L. Burnett.

We very much appreciate your assistance in this matter.

Sincerely,

James S. Kane

James S. Kane
Associate Director
for Basic Energy Sciences
Office of Energy Research

Enclosure

INTRODUCTION

It is hoped that this report will prove useful as a convienent compilation and index of the projects funded in fiscal year 1980 by the DOE Division of Nuclear Sciences/Office of Basic Energy Sciences.

Attached to each summary is information regarding the category in the Federal Budget to which the project belongs, as well as the amount of operating expense funds provided in FY80. ($1 K = $1,000) The budget codes can be interpreted as follows:

-01:	Low Energy Nuclear Research
-02:	Nuclear Data Measurements
-03:	Nuclear Data Compilation and Evaluation
-04:	Heavy Element Chemistry
-02-01:	Electromagnetic Isotope Separation
-02-02:	Special Isotope Preparation

Projects funded under the first three budget categories: -01, -02, and -03 are currently managed by S. L. Whetstone, Division of Nuclear Physics; -04, -02-01, and -02-02, by J. L. Burnett of the Division of Chemical Sciences. Detailed information about a given project may best be obtained by communicating directly with the investigators listed.

It should be noted that an appreciable program of research in nuclear science (including medium-energy, heavy-ion, and nuclear theory research) is also supported by the Department of Energy in the Division of Nuclear Physics/Office of High Energy and Nuclear Physics.

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TABLE OF CONTENTS

SECTION A

Page

Laboratories

Ames Laboratory 1
Argonne National Laboratory 2
Brookhaven National Laboratory 6
Idaho National Engineering Laboratory 10
Lawrence Berkeley Laboratory 11
Lawrence Livermore Laboratory 17
Los Alamos Scientific Laboratory 18
Oak Ridge National Laboratory 22
Pacific Northwest Laboratory 35

SECTION B

Universities

Clark University 36
Colorado, University of 37
Colorado School of Mines 38
Cornell University 39
Denison University 40
Duke University 41
Florida State University 42
Georgia Institute of Technology 43
Iowa, University of 44
Iowa State University 45
Kentucky, University of 46,47
Lowell, University of 48
Maryland, University of 49
Massachusetts Institute of Technology 50
Michigan, University of 51,52
Middle Tennessee State University 53
New Mexico, University of 54,55
New York, City University of/Brooklyn 56
New York, State University of/Albany 57
North Carolina, University of/Chapel Hill 58
North Carolina State University 59,60
Ohio University 61
Oklahoma, University of 62
Pennsylvania, University of 63
Princeton University 64
Rensselaer Polytechnic Institute 65
Tennessee, University of 66,67
Tennessee Technological University 68
Texas A&M University 69,70

Page

Washington, University of 71,72
Wisconsin, University of 73,74
Yale University 75,76

SECTION C

Others

National Bureau of Standards 77
Rockwell International 78
SRI International 79

SECTION D

Index of Investigators 80

SECTION E

Index by Budget Categories 83

LABORATORIES

Ames Laboratory -01 $190 K
Iowa State University

John C. Hill, F. K. Wohn

I. Decay of Fission Products. The major thrust in our program is the study of the decay of neutron-rich nuclides produced by fission at the High Flux Beam Reactor at Brookhaven. The fission products are mass separated using the TRISTAN separator system. The elements Zn through Sr and Ag through Ba are available through use of an in-beam target ion-source combination. Measurements of γ rays, conversion electrons, and β rays are used to study nuclides with half-lives as short as a few 100 milliseconds. The above measurements establish the structure of nuclei far to the neutron-rich side of stability. At present emphasis is being placed on the study of the regions near the doubly-magic nuclei ^{132}Sn and ^{78}Ni. The results of these studies are also of interest for the design of fission reactors and modeling of loss-of-coolant accidents, since the heat distribution in the reactor core depends on the fission products available and the energies of the γ and β radiation emitted.

II. Heavy Ion Coulomb Dissociation. A search is underway for Coulomb dissociation produced by the interaction of relativistic heavy ions produced at the Bevalac accelerator at Berkeley with selected targets. The (X,Xn) reaction where X is a relativistic projectile of energy 2GeV/A ranging from p to ^{40}Ar is used to indicate the presence of Coulomb-dissociation. In this process the target nucleus is excited by photon exchange when the two nuclei are too far apart for the nuclear interaction to be significant. It is expected that if Coulomb dissociation does occur the nucleus will be excited into the giant dipole or some higher multipole resonance. The process will enable us to study the excitation of giant resonances at relativistic energies by purely electromagnetic interactions.

III. Decay of Neutron-Rich Nuclides with A<70. It is quite difficult to produce and study very neutron-rich nuclides outside the fission region. We make use of the unique flux of high-energy neutrons produced at the main beam stop at LAMPF. The nuclides of interest which are produced by spallation are separated by rapid gas-phase radiochemistry. Two new nuclides, ^{39}S($T_{\frac{1}{2}}$=11.5s) and ^{46}Ar($T_{\frac{1}{2}}$=8.9s) have been isolated and their decay schemes determined. Aside from the interest of these studies for nuclear structure considerations, the characteristics of these neutron-rich nuclides must be determined in order to model the r and s processes in stars in which the heavy elements are produced.

ARGONNE NATIONAL LABORATORY

Physics Division -01 $1365 K

Nuclear Research FY 1980

C. N. Davids, A. J. Elwyn, G. T. Garvey, W. F. Henning, R. E. Holland, R. J. Holt, H. E. Jackson, Jr., V. E. Krohn, W. Kutschera, R. D. McKeown, F. P. Mooring, L. Meyer-Schutzmeister, J. E. Monahan, G. R. Ringo, J. P. Schiffer, R. K. Smither, J. L. Yntema.

I. Neutron Electric Dipole Moment. The existence of a nonvanishing neutron EDM would challenge the fundamental symmetries under space inversion and time reversal. Its magnitude would test gauge theories of the weak interaction. This experiment will measure the EDM by observing the effect of an electric field on the precession of bottled ultracold neutrons. The anticipated sensitivity in the current phase of the experiment is 1×10^{-25} e-cm.

II. Photonuclear Research. Includes non-El giant resonance phenomena, basic reaction mechanisms in light nuclei, fundamental properties of the deuteron, and photon scattering experiments to study couplings between collective excitations in medium and heavy nuclei. The major effort in FY 1980 is dedicated to accurate neutron-polarization measurements in deuteron photodisintegration.

III. Weak Interaction Research. The nucleus is used as a laboratory to study fundamental symmetries of the weak interaction. Experiments includes tests of the conserved vector current hypothesis and the existence of second-class currents. The main present effort is a search for parity violation in the reaction $^{6}Li(\alpha,\gamma)^{10}B$, using a polarized ^{6}Li target.

IV. Charged-Particle Reactions and Radioactivity. Includes reactions of ^{6}Li and ^{7}Li of interest for "exotic" fusion power cycles, $^{4}He(^{3}He,\gamma)$ reactions related to the solar neutrino problem, isotopes of interest to nucleosynthesis, gamma-ray studies of mirror nuclei in the $f_{7/2}$ shell, and other nuclear structure experiments. A new helium jet recoil transfer system is being developed for fast radioactivity experiments.

V. Accelerator Mass Spectrometry and Archaeological Dating. The FN tandem is used with a magnetic spectrograph to measure isotope concentrations in the range 10^{-8} to 10^{-14}. This technique has been used to measure radioactive half lives in the range 10^{2} to 10^{6} years, cross sections for producing isotopes of astrophysical interest by proton bombardment, and for highly efficient measurements of ^{14}C concentrations for archaeology. Feasibility studies for using the picosecond pulsing of the superconducting linac for mass spectrometry by time-of-flight are under way.

VI. Laser Fluorescence Spectroscopy. A facility is being developed with a cooled He jet for measuring isotope shifts and hyperfine interactions by Doppler-free laser fluorescence spectroscopy, using beams from the superconducting linac.

VII. Accelerator Operations. We operate a Tandem-Linac facility (a modified FN Tandem with a picosecond-pulsed superconducting linac energy booster), and a high-current single-ended 4 MV Dynamitron accelerator. About one fourth of the beam time of these accelerators is used by groups including university-based researchers.

LABORATORIES

Argonne National Laboratory -01 $565 K
Chemistry Division

Nuclear Research

B. B. Back, R. R. Betts, J. E. Gindler, L. E. Glendenin, B. D. Wilkins, K. L. Wolf, A. M. Friedman, I. Ahmad, R. R. Chasman

Nuclear research supported activities in the ANL Chemistry Division include studies in nuclear fission and the nuclear structure of actinide nuclei. The nuclear fission research program is directed toward achieving a fundamental understanding of the nature of the fission process. The dependence of various aspects of the process (e.g., fissionability, fragment mass and angular distributions, kinetic energy release) on the structure, excitation energy, and angular momentum of the fission system provide fundamental information on the location of nuclear shells and on the rigidity of nuclei against centrifugal stress. Fusion and transfer reactions with both light and heavy-ion projectiles at the ANL tandem-superconducting linac, as well as the accelerators at LBL, ORNL and Michigan State University, provide a controlled and separate variation of excitation energy and angular momentum over a broad range for these studies. The current primary emphasis of the nuclear structure research program is on a search for parity doublets in the light actinides which are predicted to exist as a result of strong octupole correlations. If observed, such doublets may provide a unique tool for the study of parity-violating interactions.

LABORATORIES

Argonne National Laboratory -02 $120 K
Chemistry Division

Nuclear Data Measurements

L. E. Glendenin, J. E. Gindler, D. Henderson

The purpose of this nuclear measurements program is to augment the fission yield data base by determining fission product yields (mass distributions) for monoenergetic-neutron-induced fission of the fissile and fertile nuclides of importance in the ^{238}U-^{239}Pu and ^{232}Th-^{233}U fast-reactor breeding cycles. Knowledge of fast-neutron fission product yields is important to many aspects of reactor technology including design and operation of reactors, dosimetry, fuel reprocessing and management of radioactive waste. The fission yields are determined by radiochemical and γ-ray spectrometric measurements of the fission products in targets irradiated with monoenergetic neutrons in the energy range of 0.1 to 8 MeV provided by the ANL fast neutron generator facility. The systematics of the experimental fission yield data can then be used to calculate mass-yield distributions for fissionable nuclides irradiated with fast neutrons of a given spectral shape characteristic of a particular set of fast reactor conditions. Fission yield systematics from this program also add to our fundamental knowledge of the nuclear fission process by furnishing basic information on the dynamics of the descent from saddle to scission point, in particular on the unresolved question of how much of the potential energy release appears as nuclear dissipation energy associated with viscous heating.

LABORATORIES

Argonne National Laboratory -04 $960 K
Chemistry Division

Heavy Elements Chemistry Research

W. T. Carnall, J. V. Beitz, J. P. Hessler, L. Morss, J. C. Sullivan, F. Wagner, Jr., D. W. Wester

Heavy element research at Argonne encompasses programs in both the chemistry and physics of the actinide and lanthanide elements. Efforts in solution, solid state, and photochemistry interact closely with more physically oriented program segments where mechanistic studies of energy transfer and excited state relaxation are emphasized.

While the thrust of the research is fundamental in nature, there is a clear potential in each program element for important contributions to more applied areas of the energy development mission of DOE. An understanding of the electronic structure of the actinides in their different valence states is basic to the interpretative needs of the program. A broad effort in atomic and crystal spectroscopy that has both a strong experimental and theoretical orientation is making steady progress in developing the required energy level analysis.

Existing unique facilities for pulse radiolysis make it possible to probe the course of oxidation-reduction reactions of actinides in solution over the whole range of possible valence states. Electrochemical and laser-excitation techniques are adding new dimensions to these studies, particularly in bicarbonate buffered solutions which model the aquatic environment. Volatile compounds and complexes containing the lanthanides and actinides represent potential optical gain media whose excited state relaxation characteristics are being characterized. Volatile actinide species are also the focus of the developing photochemistry effort. Programs in solid state chemistry probe the nature of actinide-oxygen interactions and their role in determining the structure and stability of complex oxyanion phases. These and other areas of the research are conducted jointly with personnel in cooperating divisions where photoelectron, Mössbauer, and extended x-ray fine structure spectroscopy facilities provide the opportunity to gain unique and complementary insights into structural relationships.

LABORATORIES

Brookhaven National Laboratory -01 $2027 K
Department of Physics

Neutron-Nuclear Research

R. E. Chrien, W. R. Kane, R. F. Casten, M. L. Stelts, H. I. Liou, D. D. Warner, R. Gill, M. Shmid, and G. Gowdy

The Brookhaven High Flux Beam Reactor, HFBR, provides a number of unique and powerful beams for neutron cross section studies, nuclear structure measurements, and fission product activity experiments. These studies are of interest to pure and applied physics.

Neutron Cross Sections. Neutron-induced reactions can be investigated at the HFBR from the thermal neutron region to energies of a few kiloelectron volts. Cross sections are measured directly by time-of-flight or diffraction techniques, or by activation through transmission filters. Because neutrons accompany the production of energy in fusion or fission processes, detailed knowledge of these neutron cross sections is of importance in energy applications.

Nuclear Structure Studies. Experience with the capture of slow neutrons shows that they are capable of populating a wide variety of final states of differing nuclear configurations by the emission of electromagnetic radiation. Neutron capture thus offers a powerful tool in nuclear structure studies. Primary and secondary gamma-ray transitions following capture provide information for assigning the quantum numbers and energies of levels in the residual nucleus. Neutron beams at thermal, resonance, and kiloelectron volts energies provide complementary information by populating states of different spin-parity range. Extensive tests of nuclear models which depend on detailed information of these levels, are being carried out.

Fission Product Studies. Neutron-induced fission leads to radioactive nuclei, or fission products, which contain an excess of neutrons as compared to stable nuclei of the same mass. The decay of these nuclei is studied by using an on-line mass separator, TRISTAN. The various radiations encountered, gamma-rays, beta-rays, and neutrons, provide stringent tests of nuclear structure models and mass formulas. They also provide useful information on the behavior of fission products. This information is needed to understand the use and disposal of nuclear fuels and for the dynamic behavior of reactors.

LABORATORIES

Brookhaven National Laboratory -01 $174 K
Department of Physics

Light Ions and General Nuclear Science

E. K. Warburton
D. E. Alburger

The Tandem Van de Graaff facility furnishes high energy beams of light ions ($A \leq 4$) of high quality which makes it possible to conduct a research program in nuclear physics interrelating with that of the heavy ion program. The emphasis is often focused on obtaining information on properties of individual nuclear levels. Frequently, these studies are directed toward specific problems of fundamental nucleon interactions and weak interaction physics. Decay properties of short-lived off-stability nuclides produced by light ion bombardments are studied in parallel with the heavy-ion produced species. Studies of specific residual nuclei produced by both light- and heavy-ion induced reactions permit exploration of the same system under vastly different conditions of energy and angular momentum. The 3.5-MV Van de Graaff, a useful adjunct to the Tandem nuclear physics program, is used occasionally for investigation of weak interactions via β-decay and has been useful in the testing of equipment and targets.

LABORATORIES

Brookhaven National Laboratory -01 $121 K
Department of Chemistry

Nuclear Spectroscopy

Y. Y. Chu, J. B. Cumming, P. E. Haustein, S. Katcoff

Investigations of the decay of radioactive nuclei, particularly those which are located far from the line of beta stability are carried out to provide the detailed spectroscopic information essential for understanding nuclear structure. Various models are being tested and new data are being provided for nuclear mass surface delineation, beta-delayed neutron emission systematics, and fission product and heavy element structure.

Studies are currently centered in three mass regions, each of which is accessible at one of the Laboratory's facilities: (1) At the unique Medium Energy Intense Neutron facility (MEIN, based on the AGS Linac) new neutron-rich isotopes of uranium, neptunium, radium, and other heavy elements are being studied. A large proportion of the nuclear data in this important region can be obtained only by radiochemical methods. (2) Neutron-deficient nuclei in the mass range from 80 to 100 which lie along the N = Z line are being studied through the use of a helium-jet system at the BNL Van de Graaff laboratory and the LBL 88-inch cyclotron. This region is characterized by rapid changes as one moves from strongly deformed nuclei with N = Z = 40 to quasispherical ones in the vicinity of doubly magic ^{100}Sn. These are reflected in both perturbations on the nuclidic mass surface and in a variety of spectroscopic features, e.g., the trend away from complicated multi-nucleon configurations to simple shell model-like ones. (3) At the TRISTAN-II on-line isotope facility (HFBR) contributions are being made to a broad program for study of the highly neutron-rich fission products. The initial experimental program will emphasize systematic conversion electron measurements of fission product nuclides as a means of elucidating spins and parities of nuclear levels.

The determination of half-lives in the region between 10 and 1000 years is another part of this program and a specially fabricated differential proportional counter permits relatively rapid estimates of half-lives in this poorly known region.

LABORATORIES

Brookhaven National Laboratory -03 $1138 K
Department of Nuclear Energy

NATIONAL NUCLEAR DATA CENTER

S. Pearlstein, C. Dunford, M. Bhat

The National Nuclear Data Center (NNDC) is responsible for the performance of four related data compilation, evaluation and information service functions: (1) the bibliographic indexing of the literature on neutron and charged particle physics investigations, (2) the compilation of experimental data resulting from those investigations; (3) the coordination of neutron, charged particle, nuclear structure and radioactive decay data evaluation; and (4) the centralized dissemination of stored information on the bibliography, experimental data and evaluated data for neutron, charged particle and nuclear structure physics.

Data from neutron and charged particle measurements performed in the U.S. and Canada are collected by scanning all the pertinent journal and report literature; attending professional meetings; visiting the important data-producing laboratories; and by corresponding by telephone and letter when necessary. Information is also collected from other U.S. centers and foreign scientists through cooperative arrangements with the international data centers maintained by the International Atomic Energy Agency (IAEA) in Vienna, Nuclear Energy Agency (NEA) near Saclay, and the USSR in Obninsk. The NNDC is responsible for solving all technical problems relating to the content and format of bibliographic and experimental data exchanged with other centers and for the computerization of data libraries.

The NNDC assists applied and basic research scientists by coordinating interlaboratory groups of experts in the distillation of experimental data to provide recommended values for nuclear data. There are two major efforts coordinated by the NNDC: (1) The Cross Section Evaluation Working Group, consisting of representatives from over 20 U.S. laboratories, meeting biannually to develop an internationally recognized data base for nuclear energy applications; and (2) the U.S. Nuclear Data Network, consisting of low energy nuclear physics information centers, meeting biannually to develop an internationally recognized data base for nuclear energy research. These coordinated efforts unite and integrate data compilation and evaluation efforts to achieve maximum utilization of manpower.

A file of requests for measurements is maintained at the NNDC to support the Department of Energy (DOE) Nuclear Data Committee (DOE/NDC) reviews of such material. The NNDC publishes the U.S. Compilation of Requests for Nuclear Data and also transmits contributions to the Worldwide Request List (WRENDA), the compilation of worldwide requests.

LABORATORIES

-03 $115 K
-02 $ 95 K
-01 $ 40 K

Idaho National Engineering Laboratory
EG&G Idaho, Inc.

Nuclear Data Measurement and Evaluation

R. L. Heath, C. W. Reich

I. Nuclear-Data Evaluation for the Nuclear Data Sheets. As one of the groups participating in the International Nuclear Structure and Decay Data Evaluation Network, this program is responsible for the ten mass chains in the region $153 \leq A \leq 162$. To achieve a four-year cycle time on all mass-chain evaluations, for publication in the Nuclear Data Sheets, this requires completion of two to three A-chains per year.

II. Radioactive-Nuclide Decay Studies. This phase of the program involves measurement of radioactive-nuclide decay properties of interest to basic low-energy nuclear-structure physics and relevant to various activities in Nuclear Sciences. Current emphasis is on the investigation of selected nuclides in the mass region $A \leq 230$, to provide information on the level properties of nuclei which lie near the beginning of the actinide region of strongly deformed nuclei. This work is related to the IAEA Coordinated Research Program on the Measurement of Transactinium Isotope Nuclear Decay Data. It involves the measurement of highly precise decay data for a number of actinide isotopes important for fast-reactor fuel-cycle and materials safeguards applications. The INEL contribution to this Program is the measurement of precise gamma-ray intensities.

III. Neutron-Capture Gamma-Ray Spectroscopy. This activity involves the study of the primary and secondary gamma-ray transitions emitted following neutron capture as a means of investigating the low-energy level structure of selected nuclides. Studies involve the use of the 2- and 24-keV "filtered" neutron beams from the HFBR at BNL to provide "resonanced-averaged" primary capture gamma-ray spectra.

IV. Delayed-Neutron Spectroscopy. A program to measure the spectrum of delayed neutrons emitted from individual fission-product nuclides has been initiated. Fission-product isotopes are produced "on-line" using the TRISTAN isotope-separator facility located at BNL. Proton-recoil counter techniques will be employed to measure the neutron spectra in the energy region between a few keV and a few hundred keV. Data presently available in this energy region are deficient.

LABORATORIES

Lawrence Berkeley Laboratory
Nuclear Science Division

-01 $213 K

Nuclear Reactions

J. Cerny, H. E. Conzett

This light ion research program has utilized 40-100 MeV ^{3}He beams and the on-line mass analysis system RAMA at the 88-inch Cyclotron to discover three beta-delayed proton emitters: ^{20}Mg, ^{24}Si, and ^{36}Ca. RAMA employs a helium jet to transport activity via skimmers to a hollow cathode ion source. Activity is extracted, mass separated and deposited on thin foils or on a magnetic tape system in the analyzer focal plane. Discovery of these nuclides, which is only made possible by providing a low background environment via mass selection, completes three isospin quintets whose members are all bound to isospin-allowed particle decay modes and provides a significant new test of the isobaric multiplet mass equation for quintets. Many unknown, proton-rich light nuclides (e.g. ^{22}Al, ^{35}Ca) with highly unique properties remain to be discovered and can be produced best by the high energy p and ^{3}He beams available at the 88-inch Cyclotron. Other light ion studies involving exotic reactions, such as (^{4}He,^{2}He) investigations, have led to the identification of two-neutron, high spin states in nuclei throughout the 1p and 2s1d shells.

Spin-dependent interactions in nuclear reactions and scattering at incident proton and deuteron beam energies from 15 to 60 MeV are also studied. This important energy region is largely unexplored since it is inaccessible to the polarized beams from tandem accelerators. Current projects include: 1) Measurements of the various polarization observables in pd scattering for comparison with exact three-nucleon calculations. 2) An accurate model-independent determination of an important deuteron D-state parameter from measurements of the cross section and tensor analyzing power in $\vec{d}$p scattering. 3) Experiments which display uniquely the operation of a basic symmetry property of the nuclear interaction. Two of the fundamentally important experiments of this nature being pursued are: i) a determination of the weak-interaction parity violating part of the nucleon-nucleon force from a measurement of the longitudinal analyzing power in $\vec{p}$p scattering at 50 MeV, and ii) a test of the principle of time-reversal invariance in nuclear reactions from measurements of the analyzing-power and the polarization in a reaction and its inverse, respectively.

LABORATORIES

Lawrence Berkeley Laboratory -01 $55 K
Nuclear Science Division

Fission and Heavy Ion Studies

L. G. Moretto

Our fission program is a subset of our broader field of research, namely heavy ion reactions. Several aspects of the fission process are being considered. a) Direct fission vs. ordinary compound nucleus fission. There is evidence that a fission-like component present in many heavy ion reactions may not arise from compound nucleus formation. If this is the case, neutron decay competition should be absent. The angular momentum distribution associated with the fragments as determined by measuring the dependence of the gamma-ray multiplicity vs. mass asymmetry should reveal whether there are neutron emission and other competing channels or whether there is indication of direct fission. b) Sequential fission decay after deep inelastic processes is used to determine the degree of alignment of the fragment spin. A complete theory for the in- and out-of-plane angular distributions has been developed including the essential dependence of the fission decay width upon angular momentum. c) It is commonly stated that an increase in angular momentum increases the fission probability. We have found that for large fissionability parameters this is not the case. At large angular momenta an enhancement of alpha decay is to be expected as compared to both fission and neutron emission.

LABORATORIES

Lawrence Berkeley Laboratory -01 $600 K
Nuclear Science Division

88-Inch Cyclotron Operation

B. G. Harvey

The 88-Inch Cyclotron is a variable energy isochronous cyclotron with spiral ridge focussing. Maximum energies for the accelerated particles are 60 MeV for protons, 65 MeV for deuterons, 130 MeV for alpha particles and 145 MeV for ^{3}He. Intensities of the light ions are limited by the deflector to about 3000 watts of power output; polarized beams are limited by source intensities. Ion sources for the cyclotron include filament arc sources for light ions and an axially injected polarized proton and deuteron source. The axial injection line has the capability of injecting other charged ions prepared in an external source. The project operates, maintains, and improves the cyclotron and beam transport facilities up to the experimental areas, maintains the building and shop facilities, and coordinates machine use by local and outside experimenters. The cyclotron operates 20 eight-hour shifts per week for in-beam experiments in nuclear chemistry and physics, isotope production and beam development.

There are some ongoing experimental programs at the 88-Inch Cyclotron which do not qualify as basic nuclear research. They collectively use $\leq$6% of the total available beam time and are encouraged because thay all represent good science with application, in many cases, to urgent national problems. Many of these projects also make good use of the unique capabilities of the Cyclotron. Curie quantities of the positron emitters ^{11}C and ^{13}N are produced for tagging amino acids such as valine or dihydroxyphenylalanine for evaluation of pancreas, myocardial and brain metabolism. Bombardments of d/l leucine with polarized protons are being made in a search for the origin of the left-handedness of the amino acids, basic constituents of living organisms. Biomedical work at the cellular level includes radioprotection, LET studies and exposures at relatively low nuclear fragmentation. Large scale production of ^{18}F is being developed, and recoil ^{18}F atoms are being used to label glycine in compounds for possible use in nuclear medicine. Random bit errors induced by cosmic rays in computer chips used in satellites are being studied with heavy ion beams, which are also used to calibrate detection instruments for the satellite work. In other studies, the amounts of low Z elements in atmospheric aerosols are being determined by charged-particle induced reactions, and meteorite formation is being investigated with in situ determinations of the micro-distributions of Bi and Pb in unequilibrated ordinary chondrites.

LABORATORIES

Lawrence Berkeley Laboratory -01 $337 K
Nuclear Science Division

Nuclear Instrumentation and Advanced Detector Systems

F. S. Goulding, C. R. Gruhn

I. Instrumentation for Nuclear Science. Three main functions are performed: (i) maintaining all general purpose electronic instruments including data acquisition and processing systems used by the Nuclear Science Division, (ii) developing special purpose instruments and hardware associated with general divisional systems, and (iii) carrying out hardware research and development aimed toward long term needs.

II. Detector Research and Development. A liquid Xe ionization chamber has been designed as a prototype for a liquid Xe detector ball to be used as a 4π γ-ray detector. The goal is to achieve a resolution of 30 keV FWHM on 1 MeV γ-rays but substantially better results are theoretically possible. Such a detector would exhibit an energy resolution intermediate between that of germanium and that of scintillation detectors.

III. Advanced Detector Systems. This project is aimed toward improvements in semi-conductor detectors for use in a broad range of nuclear experiments of interest to many laboratories in the United States. The effort is split between some work designed to elucidate radiation-damage effects and mechanisms in high-purity germanium detectors and considerable work on detector technology. Recent radiation damage work has included studies of both neutron damage and of damage induced by high-energy charged particles in high-purity germanium detectors. As might be expected, the character of the damage, such as its annealing behavior as a function of temperature, is quite different in the two cases and is still under investigation. High purity germanium detector development is concentrated on the problems of producing reliable thin n^+ contacts (made by phosphorous or arsenic ion-implantation) and on provision of good surface protection to make the detectors relatively insensitive to ambient contaminants. The development of hydrogenated-amorphous germanium sputtered coatings has successfully solved the protection problem. Very large-area (5 and 7 cm diameter) lithium-drifted silicon detectors have been developed for use in detector telescopes for long-range particle spectroscopy and ion-identification. Some of these detectors have extremely uniform thickness (<10μm variation in 5 mm total thickness) and thin dead layers (<10μm), while others are position-sensitive devices.

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LABORATORIES

Lawrence Berkeley Laboratory -03 $235 K
Nuclear Science Division

Isotopes Project

Janis M. Dairiki

The Isotopes Project compiles and evaluates nuclear structure and decay data. From 1940-1978 the project had as its main objective the production of the Table of Isotopes; the seventh edition, published in 1978 by John Wiley, is the last of the series. This comprehensive data compilation is used both in nuclear applications and in basic research; 5000 copies of the seventh edition have been sold in the first year. The project also compiles and publishes the Table of Nuclear Moments, the only such table maintained on a continuing basis. The most recent version was published as an appendix in the seventh edition of the Table of Isotopes. Extensive computer programs have been developed since 1971 to expedite the handling and storage of data and to aid in the selection, editing and convenient final presentation of the data for publication.

The size of the evaluation task has increased dramatically with the exponential growth in the volume and complexity of experimental data. In order to avoid costly duplication, the Isotopes Project now coordinates its evaluation efforts with those of other data centers through both an international data network and the U.S. Nuclear Data Network (NDN), under the management of the National Nuclear Data Center (BNL). The evaluation of 28 mass chains (A = 167-194) with a 4-year cycle time has been assigned to the LBL group as a principal responsibility. Evaluated mass-chain data from all network members are maintained in an internationally recognized database, the Evaluated Nuclear Structure Data File (ENSDF), and are published in Nuclear Data Sheets.

The Isotopes Project has been asked to produce, on behalf of the NDN, a Radioactivity Handbook for applied users. Data will be taken from the ENSDF file. The Handbook is scheduled to be published at four-year intervals, beginning in 1982.

LABORATORIES

Lawrence Berkeley Laboratory -04 $915 K
Materials and Molecular Research Division

Actinide Chemistry

Norman Edelstein

The basic purpose of this project is to study actinide materials in order to provide the basic knowledge necessary for their safe and economic utilization in present day and future technology. This program includes studies of the preparation and physical and chemical properties of a variety of new gaseous, liquid, and solid phases. Synthesized compounds will be characterized by x-ray diffraction, optical and vibrational spectroscopy, and magnetic resonance and magnetic susceptibility techniques. Equilibrium constants for complex formation will be measured. From the complementary studies, new insights into the structural and chemical principles of actinide compounds will be gained to imagine new bonding situations and to design new synthetic schemes to produce new materials.

A major aspect of the program is concerned with the design of sequestering agents for the actinide ions (in particular plutonium (IV)) which can engulf such ions. These compounds are intended to be used in the treatment of actinide poisoning as well as for possible applications in the treatment of spent nuclear reactor fuels. The preparation, structural, and physical studies of new types of organoactinide, related organolanthanide, and new actinide inorganic complexes (such as the borohydrides) will continue to be studied. Studies on the optical spectra of free atoms and ions, and on actinide ions in crystals and in molecular compounds, will be pursued with emphasis on free ions which have the same oxidation state as found in chemical compounds.

LABORATORIES

	-02	$150 K
	-01	$150 K
Lawrence Livermore National Laboratory	-02	$150 K

Studies of (n, charged particle) Reactions with 14-15 MeV Neutrons

R. C. Haight, S. M. Grimes, and H. H. Barschall

Materials bombarded by fusion neutrons are altered by nuclear transmutations that produce hydrogen and helium. To assess the potential performance of these materials for fusion reactor application, cross section data are required by the fusion community and the Office of Fusion Energy. Under the sponsorship of the DOE Office of Basic Energy Sciences, we measure these quantities by detecting the charged particles emitted by materials under bombardment by neutrons of 14 to 15 MeV. By also measuring the energy and angular distributions of the charged particles, we are able to test nuclear reaction theories through model calculations and to deduce KERMA factors for consideration of energy deposition by the neutrons.

R. J. Borg, M. Lindner, and D. A. Leich

Nuclear Astrophysics. It is widely believed that the β^- decay of ^{187}Re provides the most reliable nuclear chronometer for dating the age of our galaxy. However, the half-life of this isotope is not reliably known. Our program is the direct experimental measurement of the decay rate by measuring the production of ^{187}Os from chemically pure Re.

R. A. Meyer, E. A. Henry, and G. L. Struble

Study of Isotopes Important to the Reactor Decay Heat Problem. We use rapid, automated, nuclear-chemistry techniques to isolate and study short-lived fission products. This method isolates isotopes of a particular atomic number rather than mass number in contrast to on-line mass-separation techniques. With the chemical method, it is often possible to enhance a particular isotope by a sequency of timed, chemical-separation steps. We use two techniques for chemical isolation of fission products: autobatch and continuous. In the former a computer-controlled batch chemical system is integrated with our spectroscopy equipment and performs chemical separations within times as short as one second, followed by measurement and recycle within less than 30 s. The latter technique produces steady-state sources by use of gas-jet delivery of fission products, and in-flight gas-phase chemical reactions to chemically purify the desired species.

LABORATORIES

Los Alamos Scientific Laboratory
Physics Division

-02	$175 K
-01	$125 K
-02	$120 K
-02	$120 K

H. Britt, R. Brown, D. Drake, J. Gilmore, N. Jarmie, G. Ohlsen, G. Russell, J. Wilhelmy

I. Low-Energy Fusion Cross Sections. Measurements are being made of cross sections for reactions among the hydrogen isotopes ^{2}H and ^{3}H in the bombarding energy range 10-120 keV. The measurements involve a large improvement in the precision of both absolute cross section and energy determinations over previous experiments. These reactions are of fundamental importance to the understanding, design, and development of future controlled-fusion, energy-production systems. It is expected that improved cross section information will have significant impact on development in many applied fusion programs.

II. Nuclear Fission. This program has aimed primarily at using various experimental techniques to infer the properties of the nuclear potential energy surface which controls the fission process in actinide elements. Results have confirmed the influence of deformed nuclear shells on the fundamental character of fission and indicates that the underlying potential energy surface is much more complex than previously supposed. Measurements of mass and kinetic energy distributions for very heavy actinides indicate dramatic changes in scission properties for fissioning in the heavy actinide region (Cf-Fm). These changes from predominantly asymmetric to predominantly symmetric mass distributions appear to indicate the importance of nuclear shells for shapes near scission.

III. Neutron Capture Reactions. This research program investigates the neutron capture reaction both below and above the giant-dipole resonance. Measurements include the asymmetry of γ-rays for neutrons between 20 and 30 MeV to obtain evidence for the isovector quadruple resonance. On the low energy side of the giant dipole resonance, capture cross sections and angular distributions of γ-rays are being studied for both closed-shell and deformed nuclei to test the current theoretical models of the capture mechanism.

IV. Fertile-to-Fissile Conversion Program. Basic neutronics data, initiated by 800 MeV proton spallation reactions, are important to spallation neutron source development and electronuclear fuel production. The LASL Fertile-to-Fissile Conversion (FERFICON) program is a cooperative effort with the Chalk River Nuclear Laboratory. The LASL experiments provide an extension to 800 MeV of similar measurements (but more exhaustive in numbers) being conducted using the TRIUMF-Cyclotron in Vancouver, B.C. The Canadian measurements are being done at proton energies of 350 and 480 MeV. The LASL FERFICON program consists of two parts: a) determination of total neutron yields from targets, and b) measurements of fertile-to-fissile conversion efficiencies. The experiments are relevant to the above applications and provide data to validate computer codes.

LABORATORIES

Los Alamos Scientific Laboratory -03 $260 K
Theoretical Division

Physics of Production and Transmutation of Nuclei

P. G. Young, G. M. Hale, E. D. Arthur, D. C. Dodder, D. G. Madland

I. R-Matrix Theory

Development and application of R-matrix techniques are carried out to describe nuclear reactions among light elements. Emphasis is placed on interpretation and improvement of nuclear data that are used as cross section standards or that are important to fusion reactor studies, and to providing theoretical support to light element experimental programs. Mass systems presently under study include A = 2, 4, 5, 6, 7, and 11. Methods of implementing charge independence in R-matrix analyses and other basic developments are being investigated.

II. Reaction Theory Studies

Development of compound nucleus, statistical, preequilibrum, and direct reaction theory models, and studies of parameter systematics are carried out for improved evaluation and extrapolation of nuclear data. Emphasis is placed on improvement of level-density representations, direct reaction channels, gamma-ray probabilites, and fission channels in model codes used for nuclear data evaluations. Parameter optimization studies are performed with emphasis on nuclei pertinent to national energy programs. Global neutron optical-model parameters are being derived on a shell-by-shell basis and, in regions of strong nuclear deformation, the optical potential is deformed by use of the coupled-channel formalism and the collective model.

III. Fission Yield Theory

Development of fission yield theory is carried out for the purpose of deriving more reliable data. The primary goal is to apply recent advances in the understanding of the fission process up to the scission point to detailed calculations of particle-emission properties and distributions of fragments beyond the scission point. Concurrently, the phenomenological fission yield relationships utilized in ENDF/B evaluated data files will be reformulated as advances are made in fundamental yield theory.

IV. Data Evaluation

Limited support is provided to incorporate certain BES-sponsored measurements and calculations into ENDF/B evaluated nuclear data files. Current evaluation projects include development of charged-particle-induced data libraries for fusion applications based on the above R-matrix analyses and incorporation of new experimental data into the ENDF/B ^{6}Li and ^{7}Li evaluations.

LABORATORIES

Los Alamos Scientific Laboratory -01 $30 K
Critical Assemblies Laboratory

High-Pressure ^{3}He Neutron Scintillation Spectrometer

Albert E. Evans

A high-pressure (2300 psig) helium-gas scintillator cell previously built at LASL will be emptied and filled with ^{3}He gas and evaluated as a neutron spectrometer. Some experimentation with gas mixtures (a trace of Xe or other Noble gas is required) and with the reflective inner surface of the cell will be required in order to obtain optimum results. A filling manifold will have to be built to pressurize the cell and to recover and purify the ^{3}He. Tests will be conducted using monoenergetic neutrons from a Van de Graaff accelerator.

This proposal is in support of the TRISTAN project at Brookhaven National Laboratory. It was requested at a Delayed-Neutron Workshop held at Los Alamos on 3-4 January, 1980, by participants planning the TRISTAN program. It is hoped that the work will lead to the development of a fast-risetime (< 5 ns), efficient fast-neutron spectrometer suitable for n-γ and n-n coincidence spectrometry at relatively low fluxes, such as in the decay of delayed-neutron-emitting fission products.

LABORATORIES

Los Alamos Scientific Laboratory -04 $83 K
Chemistry - Materials Science Division -04 $102 K

Thermodynamics of Transplutonium Elements and Early Actinides

John W. Ward

This research program is concerned with the measurement of thermodynamic properties of actinide elements and compounds by high temperature Knudsen effusion/mass spectrometric techniques. Of particular interest are those systems for which there are at present little data (or for which the data appear unreliable). The pure metals are being examined first. Definitive values have been measured for ^{241}Am and ^{243}Am, and ^{249}Cf. Preliminary results are now being evaluated for ^{249}Bk and ^{231}Pa. Metal-oxide systems will also be studied with these techniques, as well as alloys and other compounds of interest. Combination of precise vapor-pressure values with thermodynamic functions calculated on the basis of electronic and magnetic properties allows tabulation of heats, entropies, free-energies and heat capacities from 298K to the highest temperatures of measurement. The increase in the stability of the dipositive state in the heavy actinides is being studied, utilizing vaporization techniques from appropriate liquid-metal solvents.

Chemistry of Oxo Complexes

R. A. Penneman, P. G. Eller and T. L. Cremers (Post Doc)
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Los Alamos, NM 87545

The basic chemistry of light actinides is being developed, especially the less studied valences and species of Pa and U. Specific projects include: Crystals of UO_2Cl, UOF_4; the extensive chemistry of UOF_4 and UF_5 in acetonitrile, dimethylformanide and 50 non-aqueous systems; reactions of oxy-organics with UF_6, UF_5; complex formation, ionic and molecular species stabilization; structural properties; the role played by 5f electrons; properties of Pa, d-block vs f-block character; hydrolytic behavior, binding of soft ligands; non-aqueous synthetic techniques; single-crystal x-ray diffraction and nuclear magnetic resonance; synthesis and characterization of novel light actinide compounds; (1) Isolation and characterization of MO_2^+ (M = Pa,U) species. (2) Preparation and structure of the presently unknown PaF_6 species. (3) Complexes of U(V) and Pa(V). (4) Non-aqueous chemistry of UOX_4, MX_5, MOX_3, and M(III) (M = Pa,U). (5) Crown ether chemistry of Pa. (6) Horizontal and vertical bonding comparisons.

LABORATORIES

Oak Ridge National Laboratory -01 $245 K
Physics Division

Light Ion Nuclear Physics

F. E. Bertrand

The research performed under this task is designed to elucidate excitations of the nucleus. Such excitations may be the result of collective motion in which a majority of the nucleons in the nucleus move together or the result of single-particle excitations between nuclear energy levels. Our approach to the research is designed to study both of these types of nuclear exicitations.

Through the use of inelastic scattering of intermediate-energy protons, deutrons, and alphas, we study the most extreme example of collective excitation, giant resonances. On the other hand, the (p,n) reaction is often selective in its excitation of nuclear states having simple particle-hole configurations. The use of α-particle-induced Coulomb excitation has allowed a direct measurement (transition rate) of the collectivity of nuclear levels.

This task is directly related to the other research programs of the Physics Division, which are designed to investigate nuclear properties through the use of heavy-ion and pion-induced reactions.

LABORATORIES

Oak Ridge National Laboratory -01 $550 K
Physics Division

Basic Neutron Physics Research
J. A. Harvey, D. J. Horen, C. H. Johnson, R. L. Macklin, S. Raman and G. G. Slaughter

Neutron spectroscopy is a unique technique for studying the detailed structure of nuclei at high excitation. The purpose of this program is to measure, analyze and interpret neutron cross sections, principally of enriched isotopes; for basic nuclear physics but also to be responsive to applied cross section needs for fusion and fission reactors. The measurements are made with the ORNL electron linear accelerator. It is usually necessary to make as many types of measurements as possible to understand the nature of neutron reaction mechanisms and nuclear structure. This program covers six types of experiments.

1. High-resolution differential elastic (and inelastic) scattering measurements up to ~2 MeV to determine the ℓ-values of resonances.

2. High-resolution total cross section measurements from 0.01 eV to 80 MeV to study level densities, the fragmentation of single particle states for light or near closed-shell nuclides, the more complex multiple quasi-particle nature (intermediate structure) of medium weight nuclides and s-, p-, and d-wave neutron strength functions and statistical properties of complex nuclides.

3. High-resolution gamma-ray spectral measurements from neutron capture in individual resonances up to ~50 keV to obtain a better understanding of the nature of the capturing process (i.e., compound nucleus vs semi-direct processes; also the location of E2, M1, E1 strengths) and for nuclear spectroscopy of nuclides up to excitation energies of several MeV, particularly those which cannot be studied in detail by other means.

4. Capture cross section measurements up to neutron energies of ~3 MeV of nuclides of importance in the chronology of element formation in the galaxy, of nuclides which contribute to the better understanding of the capturing process (i.e., gamma ray strength functions), and for applied needs for reactors and neutron capture cross section standards.

5. Subthreshold and threshold fission cross section and fragment anisotropy measurements on targets such as ^{232}Th and ^{231}Pa, in cooperation with Los Alamos Scientific Laboratory and Bruyères-le-Châtel to investigate the shape of the potential energy surface and the nature of strongly deformed states trapped in a possible third minimum of the fission barrier.

6. Reaction cross section measurements such as the (n,α) reaction in the resonance energy region to learn about the nature of the processes and possible intermediate structure; also accurate (n,α) measurements on ^{6}Li to establish it as a standard for keV neutron fluxes.

LABORATORIES

Oak Ridge National Laboratory -02 $390 K
Physics Division

Actinide Neutron Cross Sections
J. W. T. Dabbs, C. H. Johnson, L. W. Weston, J. A. Harvey, M. L. Williams and S. Raman

This program's primary goal is to obtain accurate differential (i.e. as a function of neutron energy) neutron cross sections (fission, capture and total) for all actinide nuclides which occur in fission reactors, so the behavior of reactors can be predicted with a high degree of confidence under all circumstances. A secondary goal is to permit predictions of the amount of the various nuclides which will be produced under all conditions of reactor operation. This is basic to any realistic assessment of the problems involved in handling, shipping, storing, safeguarding, and (possibly) reprocessing of spent fuel.

1. This work includes differential neutron fission, capture and total cross section measurements on U, Np, Pu, Am and Cm isotopes and on other nuclides as required. The choice of measurements is on the bases of need, quality of existing data, and feasibility.

2. An important aspect, recently added to the program, is the analysis of a number of actinide samples irradiated in EBR-II for 5 years ending in 1970. The results of these analyses will serve as a cross-check on the accuracy of calculations based on the differential data. A discrepancy of a factor 2 has already been found in the first sample.

3. Sensitivity and uncertainty analyses are used for supplemental analysis of the results and to help guide the program.

4. An "Actinide Newsletter" is published annually (3 issues so far) for the purpose of improving world-wide coordination of actinide research.

LABORATORIES

Oak Ridge National Laboratory -02 $1150 K
Engineering Physics Division

Operations - Oak Ridge Electron Linear Accelerator
J. A. Harvey, R. W. Peelle, T. A. Lewis, H. A. Todd, R. G. Alsmiller

The task of the Oak Ridge Electron Linear Accelerator (ORELA) is to provide the best feasible pulsed neutron source for neutron cross section measurements over the entire neutron energy region of importance to fusion and fission power systems and of interest for low-energy nuclear physics studies. For a great share of the cross sections being studied, an electron linac like ORELA is the best type of accelerator. Neutron cross section measurements made by the time-of-flight method require an intense pulsed-neutron source which is provided here by a high-current, short-burst electron beam incident on a high-Z target surrounded by a moderator. The short-burst performance of ORELA remains the best available anywhere in the world, although the linacs at BCMN in Geel, Belgium and at AERE-Harwell in England have been replaced with units of comparable power. The design of ORELA with 11 flight paths radiating from an evacuated target room makes possible simultaneous use by many experimenters, a feature which greatly increases the total output and cost effectiveness of the facility. ORELA is used by experimenters of the Physics, Engineering Physics, Solid State, and Chemistry Divisions of ORNL and by other DOE-supported nuclear physicists for accurate high-resolution neutron cross section measurements in the energy range from ~0.01 eV to 80 MeV. The measurements are directed toward the high priority needs for neutron cross-section data for controlled fusion and fission reactor designs, to the establishment of neutron cross section standards, to provide cross sections needed for calculating the production and burn-up of actinides in power reactors, and to the understanding of neutron reaction mechanisms and nuclear structure. Energy-dependent neutron cross sections and related measurements of almost every variety are made with this facility, including total, capture, fission, elastic and inelastic scattering, (n,p) and (n,alpha) reaction cross sections, $\bar{\nu}(E)$, and the gamma-ray spectra from capture and inelastic scattering.

In detail the task is accomplished by a program of aggressive operation and maintenance of the existing linear accelerator and a companion development effort to improve the performance, reliability and versatility of the machine for the needed experiments. The most far-reaching current efforts involve improvement in electron gun design and operational use of a prebuncher to narrow the overall charge pulse injected into the accelerator waveguide.

LABORATORIES

Oak Ridge National Laboratory -02 $455 K
Engineering Physics Division

Nuclear Data for Fusion and Fission Reactors

C. Y. Fu, D. C. Larson, R. R. Spencer

The work undertaken under this program provides some of the basic nuclear data most required for the design of nuclear power producing systems. The work is divided into two subtasks:

A. Nuclear Data for Fusion Energy. The Oak Ridge Electron Linear Accelerator, ORELA, is used to obtain neutron interaction cross sections, including gamma-ray production, for nuclides of interest over the complete energy range of interest to prospective fusion energy devices. Work concentrates on nuclides, partial cross sections and energy regions unique to fusion energy applications and unlikely to be obtained in other ongoing programs. Experimental work at present concentrates on neutron and gamma-ray emission spectra and on transmission measurements. The results of the measurements are incorporated into the U. S. national reference evaluated data file system, ENDF/B, so that they become directly usable in fusion energy system applications. Evaluation for the fusion system materials C, F, Sc, Fe, Cu, and Pb are performed under this subtask for the ENDF/B system. In order to provide the correct method of interpolating and extrapolating the experimental data for the evaluations, theoretical model codes are developed and used.

B. Nuclear Data for Fission Systems. The average number of neutrons emitted in the neutron-induced fission of the fissile isotopes is the most important parameter required in the design of fission reactors, affecting the safety, performance and economy of the reactor systems. Measurements of $\bar{\nu}$ vs neutron energy for the fissile isotopes are carried out by comparison with a ^{252}Cf spontaneous fission neutron source (ratio measurement), thus any uncertainty or error in the value of $\bar{\nu}_p$ for ^{252}Cf directly affects power reactor design. A measurement of this important standard to the desired uncertainty of ~1/4% is being completed utilizing ORELA as the neutron source for the calibration of a neutron-detecting Gd-poisoned scintillator tank. These calibrations for certain neutron angle and energy ranges are combined with neutron transport calculations of tank efficiency. The successor experiments are expected to emphasize the measurement of cross sections important to improved fuel efficiency in light water reactors. The work involves development and calibration of counting devices, measurement, data analysis, and supportive neutron and gamma-ray transport calculations.

LABORATORIES

Oak Ridge National Laboratory -02 $50 K
Engineering Physics Division

Electronuclear Fuel Production Physics Studies

R. G. Alsmiller, Jr., T. A. Gabriel

The purpose of this program is to develop the medium-energy nuclear cross section data and the charged and neutral particle transport methods that are necessary for carrying out feasibility and engineering design studies for electronuclear fuel production (EFP). Because of the large amount of particle production data that is needed to carry out the design calculations, much reliance must be placed on nuclear models. Uncertainties in EFP design calculations at present are due in part to the approximate manner in which medium-energy fission is treated in the available intranuclear-cascade-evaporation models of medium-energy nuclear reactions. In this task efforts will be made to improve this aspect of the model. Careful comparisons will be made between experimental and calculated nuclear data to ensure the validity of the results obtained with the models used. Also, comparisons between results obtained with the transport methods developed as part of the program and suitable experimental data will be made to ensure the validity of the methods for design calculations.

LABORATORIES

Oak Ridge National Laboratory -02 $75 K
Health & Safety Research Division

One-Atom Detection Solar Neutrino Measurements

S. D. Kramer, G. S. Hurst, W. R. Garrett

The discrepancy between recent experimental results and theoretical calculations for the solar neutrino flux casts considerable doubt on the correctness of current theories of either stellar evolution or weak interactions. The best way to resolve this problem would be to perform additional detection experiments, using a variety of target atoms that sample neutrinos in several different energy regimes.

John Bahcall [Phys. Rev. Lett. 23, 251 (1969) and Rev. Mod. Phys. 50, 881 (1978)] has pointed out the importance of the reaction $^{7}Li(\nu,e)^{7}Be$ as a neutrino detector. Unfortunately, until now there has been now way to detect extremely small amounts of the reaction product, ^{7}Be. However, time- and spacial-coincidence techniques based on the use of resonance ionization spectroscopy in conjunction with position-sensitive proportional counters, both of which have been under extensive study at Oak Ridge National Laboratory, appear to offer a means of detecting the electron capture decay of ^{7}Be at the very low count rates characteristic of neutrino detection experiments. This or other techniques based on resonance ionization spectroscopy could also prove useful in additional solar neutrino detection reactions such as $^{71}Ga(\nu,e^{-})^{71}Ge$ and $^{81}Br(\nu,e^{-})^{81}Kr$.

LABORATORIES

Oak Ridge National Laboratory -03 $575 K
Physics Division

Nuclear Data Project

M. J. Martin

The Nuclear Data Project (NDP) is an evaluation center which, as part of the U.S. Nuclear Data Network, is responsible for collecting and evaluating nuclear structure information for 70 mass chains in the mass region A≥195.

The work involves reading and critical analysis of all literature on nuclei in the above mass region. For each research paper, the evaluators extract the data, compare them with data from other sources, and prepare critical reviews with recommended values for a wide range of nuclear structure properties. Systematic trends in these properties are investigated both as a guide in the evaluation procedure and as a means of gaining new insight into nuclear structure phenomena.

Data evaluated by the NDP are made available to both the research and the applied communities directly and through Network publication of the Nuclear Data Sheets. The NDP maintains responsibility for the scientific editorship of this monthly journal.

k Ridge National Laboratory

Transuranium Research Laboratory (TRL), Chemistry Division -04 $895 K

Chemistry of Transuranium Elements and Compounds

R. L. Hahn, R. G. Haire, J. Halperin,
L. Maya, G. D. O'Kelley, G. M. Begun

Studies of the chemical and physical properties of the 5f-actinide elements, and of the homologous 4f-lanthanides, comprise the major effort of the research program in the Transuranium Research Laboratory. Because fundamental information about the heavier actinides, from curium through einsteinium, is still relatively scarce, we determine oxidation states, redox potentials, electronic configurations, absorption spectra, crystal structures, ionic and atomic radii, thermodynamic properties, and the chemical effects of radioactive decay of these elements and their compounds. Recent results include determinations of the enthalpies of vaporization and of solution of ^{243}Am and ^{249}Cf metals; observation of a change in crystal structure of ^{243}Am metal at high pressures, > 150 kbar; measurements of the magnetic susceptibilities of ^{248}Cm, ^{249}Bk and ^{249}Cf metals and of $^{253}Es_2O_3$; and details of the chemical effects that result from radioactive decay of the tri- and di-halides in the chain, $^{253}Es \xrightarrow{\alpha} {}^{249}Bk \xrightarrow{\beta} {}^{249}Cf$.

Although much information is available for the lighter actinides, especially from uranium through americium, because of their importance in nuclear reactor technology, little data exist for them under the conditions that are expected in the natural environment and in nuclear waste repositories. We are studying these elements in solution, to identify species at very low concentrations, and to elucidate effects of pH, Eh and complexation phenomena. In research relevant to waste disposition, we have investigated the adsorption/migration of Am, Np, U, and Pu in geologic media (clays and minerals), and the effectiveness of rare earth orthophosphates (synthetic monazites) as alternate containment forms for actinide elements.

- 30 -

LABORATORIES

Oak Ridge National Laboratory
Chemical Technology Division

-02-01 $1300 K

ELECTROMAGNETIC ISOTOPE SEPARATION
E. Newman, W. A. Bell, H. R. Gwinn,
J. G. Tracy

The objective of this program is to use the calutrons to separate and provide multigram quantities of highly enriched separated stable and selected radioactive isotopes, including the actinides, to the research, commercial, and nuclear medical communities. An important aspect of the program is the research and development activities in ion source technology, beam dynamics, ion retention, and chemical recovery procedures. All isotopically enriched samples are distributed through a regular sales program or are circulated to the research community on a loan basis from the Research Materials Collection administered under the direction of DOE. In the operation of this national resource, the program is responsible for the production, distribution, quality control, and reprocessing of the material in the Research Materials Collection.

LABORATORIES

Oak Ridge National Laboratory -02-02 $2190 K
Operations Division

High Flux Isotope Reactor
J. A. Cox

The main purpose of the High Flux Isotope Reactor (HFIR) is to make research quantities of ^{252}Cf and other transuranium isotopes. These materials are produced in the flux trap in the center of the HFIR fuel element where a thermal-neutron flux of $3x10^{15}$ neutrons/cm^2·s is available to irradiate the ^{244}Cm target material. Additional irradiation facilities are also provided in the beryllium reflector to increase the production rate of the heavy isotopes.

As a secondary purpose, the HFIR has facilities for performing diverse irradiations, tests, and experiments which can benefit from the exceptionally high neutron flux available. In the fuel element flux trap a hydraulic-rabbit tube provides access to the maximum thermal-neutron flux in the reactor for short-term irradiations and other positions are ideal for fast-neutron irradiation-damage studies. The beryllium reflector contains numerous experiment facilities with thermal-neutron fluxes up to $1x10^{15}$ neutrons/cm^2·s. These facilities can accommodate either static experimental capsules or complex fuel-testing engineering loops. Four beam tubes are utilized for neutron-diffraction experiments and the installation of a small-angle neutron scattering facility was sponsored by the National Science Foundation for use by researchers from universities, industry, and other national laboratories.

The HFIR is operated to maximize the on-stream time commensurate with the requirements of the diverse irradiation programs being conducted. This policy usually results in an on-stream time in excess of 90% as is illustrated by the 91.4% attained in CY-1979 which was slightly lower than the record 94.4% attained in CY-1977.

LABORATORIES

Oak Ridge National Laboratory -02-02 $4468 K
Chemical Technology Division

TRANSURANIUM ELEMENT PROCESSING
L. J. King, F. R. Chattin, M. H. Lloyd,
J. E. Bigelow, E. D. Collins

The Transuranium Processing Plant (TRU) is the production, storage, and distribution center for the DOE heavy element research program. Since it began operations in 1966, TRU has been the only source in the United States of significant quantities of berkelium, californium, einsteinium, and fermium. TRU is a remotely-operated, hot-cell, chemical processing facility of advanced design. It functions integrally with the researchers in preparing suitable research-grade isotopes, rather than merely as a supplier. About 25 HFIR targets per year are being fabricated, irradiated, and processed to produce about 500 mg of ^{252}Cf, 50 mg of ^{249}Bk, 2.5 mg of ^{253}Es, 300 µg of isotopically pure ^{253}Es, and 1.5 pg of ^{257}Fm. Reprocessing of stored ^{252}Cf produces about 100 mg of ^{248}Cm annually. Approximately 50 shipments to researchers are made per year. These include shipments of normal production materials plus special forms and specially-prepared isotopes that were requested by researchers. The transuranium materials continue to be used nationally and internationally to study the basic chemistry and physics of the transuranium elements.

LABORATORIES

Oak Ridge National Laboratory -02-02 $27 K
Operation Division

Distribution of Special Isotopes for Research

C. L. Ottinger

Isotopes from the Research Materials Collection are distributed to DOE contractors and others performing research in which the DOE has programmatic interest. In some cases, special processing, handling, packaging, shipping, analysis, or other arrangements are required before shipment can be made. This task consists of providing such special services as needed.

LABORATORIES

Pacific Northwest Laboratory -02 $230 K
Physical Sciences Department

Fission Yield and Delayed Neutron Studies with an On-Line Mass Spectrometer

P. L. Reeder and R. A. Warner

This program provides basic nuclear data on fission yields and decay characteristics of short-lived fission products (particularly delayed neutron precursors). These basic data have applications to decay heat calculations, determination of fission product inventory, calculations of delayed neutron abundances and burnup measurements. Delayed neutron data are particularly important in reactor dynamics calculations. In addition, fission yield data are needed for comparisons with predictions of theoretical models of nuclear fission. Decay characteristics of short-lived fission products provide much information for nuclear structure theories.

Data are obtained on individual fission products produced and separated with the SOLAR on-line mass spectrometer facility. The surface ionization source used with the SOLAR facility provides ion beams of a single chemical element in contrast to ion sources currently in use at other on-line facilities. Fission yields are measured by counting individual atoms with an electron multiplier detector. Decay characteristics of short-lived fission products are measured with various beta, gamma and neutron counters and spectrometers. Some of the delayed neutron studies will be carried out at the new TRISTAN on-line isotope separator facility at Brookhaven National Laboratory.

We are currently using the short bursts of neutrons from TRIGA reactor pulses to measure the ratio of the fission yields of isomers of isotopes of Br, Rb, In, I and Cs from the thermal neutron fission of ^{235}U. These data are to be included in the ENDF/B evaluated nuclear data file for general use in fission yield calculations. Isomer yield data are important for developing theoretical understanding of how angular momentum is distributed in the fission process.

Development efforts are underway to construct a new type of neutron spectrometer with better resolution and much greater efficiency than existing ^{3}He ionization chambers. The neutron spectrometer will use gas scintillation proportional counter techniques. It will be used for measurements of energy spectra of delayed neutrons from mass separated precursors and for neutron-gamma coincidence studies.

UNIVERSITIES

Clark University
Department of Chemistry -01 $75 K

Atomic Mass Measurements and Nuclear Spectroscopy at TRISTAN

D. S. Brenner

Our research program is concerned with measuring atomic masses of short-lived, neutron-rich fission products using the TRISTAN on-line mass separator located at the High Flux Beam Reactor (HFBR), Brookhaven National Laboratory. The determination of accurate masses for neutron-rich nuclei is useful in refining mass equations which, in turn, are important for calculations related to astrophysical processes and to control and safety of nuclear reactors.

During the past year our efforts have been to (1) aid Brookhaven personnel in the installation and testing of TRISTAN at the HFBR, (2) procure, install, and make available research equipment for members of the Users' Group at the facility, and (3) develop computer software for analysis of experimental data.

In the coming year we expect to begin a program of measurements of β-ray end-point energies and nuclear decay schemes following successful demonstration of the capabilities of the TRISTAN facility.

UNIVERSITIES

University of Colorado
Nuclear Physics Laboratory -01 $685 K

J. J. Kraushaar, P. D. Kunz, D. A. Lind, R. J. Peterson, R. A. Ristinen, E. S. Rost, W. R. Smythe, C. D. Zafiratos, C. S. Zaidins

I. Direct Reaction Studies. Light ion beams from the AVF cyclotron are used to induce a wide variety of reactions, with a particular emphasis on those with outgoing neutrons. Theoretical descriptions of these reactions are developed and tested. Well understood reactions allow quantitative studies of the structure of complex nuclei. Examples include the role of the pairing interaction seen by two-nucleon transfer, shell-model states seen in single and three nucleon transfer and isospin effects studied by charge exchange.

II. Compound Reaction Studies. Collective nuclear structure is studied by the gamma and neutron decay of compound nuclei, including coincidence studies between several gamma ray or neutron detectors. Time-of-flight data are used to specify the neutron energies. Coincident gamma spectra are used to determine the level schemes of complex nuclei, with the aid of direct reaction analyses. Thermonuclear reaction rates of interest to astrophysical nucleosynthesis are measured over a wide range of energies.

III. Intermediate Energy Physics. Experimental and theoretical studies are directed towards an understanding of the mechanisms of direct reactions induced by pi mesons and energetic protons. Experiments are performed at LAMPF, TRIUMF, and the Indiana University Cyclotron Facility. As these probes are better understood they are utilized to examine previously inaccessible features of nuclear structure.

UNIVERSITIES

Colorado School of Mines
Physics Department -02 $50 K (24 mos.)

The Measurement of Total Cross Sections for Nuclear Reactions Induced by Low Energy Charged Particles

F. Edward Cecil

Scope of Work

Measurement of the total cross sections at very low energies (between about 50 and 150 keV) of a broad class of deuteron- or triton-induced one- or two-nuclear transfer reactions on light ($6 \leq A \leq 19$) targets.

The measurements will be confined to exothermic reactions with which there is an associated gamma ray (either prompt or delayed). Thick samples will be bombarded by monoenergetic beams of deuterons or tritons. Recent improved understanding of the stopping power of low energy light ions (Zeigler and Anderson, 1977) will permit the determination of the reaction cross sections from the thick target yields. The chief novelty of the measurements is their extension to unusually low energies and their consequent interest to both astrophysics and fusion energy. The deuteron measurements would be carried out on a small Cockcroft-Walton accelerator on campus, the triton measurements at the new low-energy facility at LASL.

UNIVERSITIES

Cornell University
Nuclear Science and Engineering Program -01 $80 K

Experimental Studies of Nuclides Far from Stability with the TRISTAN II Fission Product Separator at Brookhaven National Laboratory

D. D. Clark, G. S. Goldhaber

Studies will be made of the energy spectra of delayed neutron emitters and of the yrast bands of certain neutron-rich even-even nuclei.

The delayed neutron measurements will concentrate on the energy spectra in the 1- to 25-keV range and will employ time-of-flight techniques.

The yrast bands populated by the beta decay of high-spin isomers of odd nuclides will be studied via beta-gamma and gamma-gamma coincidences, and gamma-gamma angular correlations.

UNIVERSITIES

Denison University
Department of Physics and Astronomy -02 $22 K

Determination of Neutron Cross Sections and Resonance Parameters

R. R. Winters

This is a collaborative effort with ORNL staff at the Oak Ridge Linear Accelerator (ORELA). The principal investigator has just completed a sabbatical at ORNL.

Data analysis on campus is facilitated by a graphics terminal connection to a computer at ORNL.

Recent work has involved studies of neutron cross sections of the osmium isotopes in the energy region of high current interest to cosmology because of their relevance to the theory of nucleosynthesis and to determination of the age of the universe.

The ratio of the inelastic to elastic neutron scattering cross sections for ^{238}U has been measured at 82 keV, and a significantly higher value found than that obtained from earlier measurements.

Other recently published work includes measurements of the neutron capture cross sections for the palladium isotopes of particular interest as inherent poisons in fission reactors.

UNIVERSITIES

Duke University	-01	$680 K
Triangle Universities Nuclear Laboratory	-02	$220 K

E.G. Bilpuch, Director, N.R. Roberson, R.L. Walter, H.R. Weller

I. High Resolution Resonance Studies.* A variety of ultra high resolution resonance experiments are being carried out on both the 3 MV accelerator and the FN tandem accelerator. Although there is still appreciable interest in global statistical properties (strength functions, average level densities), our major emphasis is on detailed or local statistical properties. These include short and long range correlations in level spacings, and unique measurements of interference effects for reduced width amplitudes. These latter results have provided the first verification of several theoretical predictions, as well as establishing new, as yet unexplained results.

II. Radiative Capture Reactions.* The main emphasis of these studies has been to search for effects of the giant quadrupole resonances in the radiative capture reaction for a variety of nuclei. Most of the E2 effects we have observed are consistent with only direct radiation which gives a "background" which makes the observation of E2 resonances difficult. Using our high intensity polarized neutron beam, we have shown that the neutron capture reaction appears to be a more favorable tool for studying E2 resonances since the direct strength is quite small. We are also using the polarized neutron beams to pursue our interest in few nucleon systems (eg $^{3}He(\vec{n},\gamma)^{4}He$. These experiments are important since the few body problem is susceptible to "exact" calculations. We are continuing our use of proton beams from the Cyclo-Graaff (18-31 MeV) to study capture leading to highly excited bound and unbound final states. Our aim is to understand the reaction mechanism, to search for resonances built on these excited states, and to investigate the utility of "high energy" capture for studying highly excited states in the residual nuclei.

III. Neutron Polarization Studies. Models of neutron induced or neutron producing reactions contain terms for the nucleon-nucleus spin-orbit and isospin interactions. In the neutron polarization research we are now able to set new limits on the strength of the spin-dependent parts of both the central and isospin potentials. Much of the research utilizes the one newly developed pulsed-polarized charged particle beams either to induce (p,n) reactions or to produce secondary beams of pulsed-polarized neutrons for neutron scattering studies in the region between 8 to 14 MeV, an energy range that heretofore has been moderately unexplored. The spin-orbit interaction is being studied for the entire range of nuclei in the periodic table in order to complement comparable work for proton scattering.

IV. Neutron Cross-Section Studies.* Measurements of the interaction of neutron beams with a wide range of elements has been a major program at our laboratory for several years. One emphasis has been on the elastic scattering of neutron beams to permit development of more accurate nuclear models and also to provide accurate data for the design of fusion-energy sources. The second emphasis is to obtain information on the emission spectrum of secondary neutrons that are emitted when high-energy neutrons impinge on various isotopes that may comprise containment vessels or blankets for fusion-energy devices. The data is combined with theoretical models to generate better descriptions for inelastic neutron interactions. The energy of the incident neutrons in both of the above studies is 8 to 14 MeV, a region where neutron data of this type has been scarce.

*These projects are done in collaboration with faculty members from North Carolina State University.

UNIVERSITIES

Florida State University
Department of Chemistry -04 $70 K

Research in Nuclear Chemistry

Gregory R. Choppin

The primary purpose of this program is the study of the species formed by the actinide (5f) elements in aqueous solution. Parallel studies are conducted on the chemically similar lanthanide (4f) elements to gain further understanding of actinide properties by use of techniques not available for actinide studies. Potentiometry, calorimetry, visible spectroscopy, nuclear magnetic resonance spectrometry and solvent extraction are the techniques used to characterize the thermodynamic and kinetic stability of complexes formed by these 4f and 5f cations with a variety of organic and inorganic ligands. One project includes characterization of inner vs. outer sphere nature of complexes of the halate and the haloacetate complexes of tri- tetra- and hexavalent actinides. The effects of enthalpy and entropy on complexation by dicarboxylate, polyphosphate (ATP), ascorbic acid and bicarbonate ligands are being investigated. These ligands were chosen to gain insight in actinide behavior in natural and biological systems. The binding of actinides by humic and fulvic acids is a continuing major effect. Humic and fulvic acids are major components of soil and serve as transport media for metal ions in fresh water systems.

UNIVERSITIES

Georgia Institute of Technology
School of Physics -01 $20 K

J. L. Wood

Nuclear Structure from Radioactive Decay. This program is aimed at making detailed and systematic studies of low-energy nuclear structure. The experimental part of the program involves gamma-ray and conversion-electron spectroscopy of mass-separated radioactive sources. These radioactive sources are produced and studied at the UNISOR facility at Oak Ridge using reactions induced by heavy-ion beams from the Oak Ridge Isochronous Cyclotron. Particular emphasis is placed on the investigation of isotopes lying for from the beta stable region: The UNISOR on-line isotope separator facility is uniquely suited for the study of low-energy low-spin states of nuclei far from beta stability in the neutron-deficient regions. These experimental measurements are combined with an extensive program in nuclear systematics to organize and interpret the level scheme data obtained. In addition, comparison with current models is made; particularly, models of particle - core coupling, model descriptions of fermion and boson degrees of freedom and their interaction, and models of excited 0^+ states in even nuclei.

UNIVERSITIES

University of Iowa
Department of Physics -01 $47 K

E. Norbeck

I. Elastic Scattering $^{6}Li + {}^{6}Li$ and $^{7}Li + {}^{7}Li$ Using 2.0 to 5.5MeV Beams. High precision measurements are made and compared with a commonly used theoretical model for nuclear scattering, the double-folding model with "realistic" nucleon-nucleon interactions. These studies provide a severe test for the model. At high energies, only the outer edge of the internuclear potential affects the scattering, but at low energies, where the wavelength is long, the model is required to predict the entire range of the potential. For high energy ^{6}Li scattering, the folding model fails, presumably because of the breakup $^{6}Li \rightarrow \alpha + d$. Preliminary results indicate that the model provides an excellent description of the scattering for energies below the threshold for breakup.

II. $^{6}Li + {}^{6}Li \rightarrow {}^{3}{}^{4}He$. This multibody process is studied experimentally and the data compared with predictions of a finite-range distorted-wave Born approximation. At low energies the most critical part of the calculation is the potential that governs the approach of the ^{6}Li nuclei. A variety of potentials can successfully predict elactic scattering, but preliminary results indicate that only the folded potential can also correctly predict the angular correlations of the ^{4}He.

UNIVERSITIES

Iowa State University
Physics Department -01 --($124 K/24 mos.)

Nuclear Size and Shape Research

D. A. Lewis

A movable laser spectroscopy system is being developed to be used at accelerator and reactor facilities for hyperfine determinations with short-lived nuclei. Experiments are planned for the ATLAS facility at Argonne National Lab and for the TRISTAN isotope separator at Brookhaven National Lab.

UNIVERSITIES

University of Kentucky
Department of Physics and Astronomy -01 $60 K

Total (p,n) and (α,n) Cross Sections for Nucleosynthesis and Nuclear Applications

Fletcher Gabbard, Robert L. Hershberger

Scope of Work

Experimental measurements of selected total (p,n) and (α,n) reaction cross sections using the University of Kentucky Van de Graaff accelerator, followed by comparisons with model calculations made for astrophysical purposes and with the results obtained from global optical potentials.

For the period of the next two years, we propose to continue systematic measurements, using thin targets of (p,n) and (α,) reaction cross-sections and reaction rates. We propose to measure total (p,n) and (α,n) cross sections for enriched targets of ^{51}V, ^{54}Cr, ^{61}Ni, ^{64}Ni, ^{65}Cu, ^{67}Zn, ^{68}Zn, and ^{75}As. The greatest source of error in this type of measurement is the determination of target thickness. In our work we are generally able to check measurements with target thickness determinations made by Rutherford scattering of protons and alpha particles in a high precision scattering chamber. The proposed measurements will be made with an absolute accuracy of $\lesssim$ 5%.

40-574 O - 85 - 19

UNIVERSITIES

University of Kentucky
Department of Chemistry -01 $30 K

Nuclear Structure Studies of Transitional Nuclei

S. W. Yates

A systematic investigation of the nuclear level structures of the stable even-mass transitional nuclei by $(n,n'\gamma)$ reaction spectroscopy has been initiated. Questions regarding the nuclear shapes and the applicability of various nuclear models for these nuclei are being addressed. The phenomenon of collective enhancements of inelastic neutron scattering cross sections and the role of nuclear deformation effects are under examination. Comparisons between population systematics of the $(n,n'\gamma)$ reaction and other reactions are made.

Studies of the stable platinum nuclei represent the first part of a comprehensive survey of this mass region. From γ-ray angular distribution and excitation function measurements, the properties of the low-lying states in ^{194}Pt have been characterized. Essentially all known levels having $I \leq 6$ below 2 MeV are observed, and spin assignments and new level placements have been made. The negative-parity states have been interpreted in terms of the semidecoupled model. The positive-parity states have been compared with asymmetric rotor, pairing-plus-quadrupole, γ-unstable, interacting-boson-approximation, and boson-expansion model calculations. Preliminary results from a similar inelastic neutron scattering study of ^{198}Pt have produced much new information on this little studied nuclide. Each of these $(n,n'\gamma)$ studies has been complemented by neutron time-of-flight measurements.

UNIVERSITIES

University of Lowell -02 $35 K

Fast Neutron Scattering Cross Section Research

L.E. Beghian, G.H.R. Kegel, G.P. Couchell, J.J. Egan, A. Mittler, D.J. Pullen, W.A. Schier, E. Sheldon

I. Inelastic Cross Sections for ^{232}Th and ^{238}U from (n,n'γ) Measurements. Inelastic Cross sections in ^{232}Th and ^{238}U have been obtained for states in the excitation energy range 0.7 - 2.0 MeV. The level cross sections have been inferred from 125° gamma-ray production measurements which employed a Ge(Li) spectrometer in conjunction with time-of-flight techniques and Compton suppression via a NaI(Tℓ) annulus. Inelastic scattering from states in the region of excitation near 1 MeV and above is an important process which contributes to the shape of the low energy spectrum in fast reactors. The high level density in this region of excitation makes direct observation by (n,n') very difficult. The excellent energy resolution attainable in gamma-ray spectroscopy makes this technique very attractive.

II. Cross Sections for ^{232}Th and ^{238}U from (n,n') Measurements. Work is in progress on (n,n') measurements for states in ^{232}Th and ^{238}U above the ground state rotational band. Using disk scatterers and the time-of-flight technique we have been able to achieve an overall energy resolution of 15 keV optimized for the detection of neutrons of 250-300 keV in energy. This allows us to study the inelastic cross sections by direct neutron measurements as a complement to our (n,n'γ) work.

III. E O Transitions in ^{232}Th and ^{238}U. In obtaining cross sections from gamma-ray data care must be taken in accounting for electric monopole transitions. We have estimated EO strengths in these nuclei by comparing cross sections obtained in (n,n'γ) measurements with (n,n') level cross sections determined by the neutron-time-of-flight method. Computer-assisted stripping of the neutron time-of-flight spectra is required to obtain individual level cross sections for most cases of interest. As a rule this method is sensitive to EO branching ratios of 20% or larger.

IV. Ring Geometry Measurements of Inelastically Scattered Neutrons for E_n <200 keV. Neutrons scattered from the ground state and inelastically scattered from the 45-keV state in ^{238}U have been measured in ring geometry for incident energies, E_n<200 keV. The time-of-flight measurement in this "open goemetry" method yields good time resolution at 50 cm flight paths.

V. Computer Simulated Time-of-Flight Spectra. We have written the computer code IMBUI to simulate neutron time-of-flight spectra for different experimental conditions. This code includes the effects of neutron target cross sections and kinematics, flight path dispersion caused by the scatterer geometry, energy dispersion introduced through the scatterer kinematics by the finite range of scattering angles, and neutron attenuation.

VI. Theoretical Calculations of Inelastic Cross Sections in ^{232}Th. The cross section data for ^{232}Th at incident energies from 0.8 - 2.1 MeV populating a variety of excited levels have been compared with the predictions of the compound-nucleus (CN) model using appropriate optical potential parameters. With increasing projectile energy, the CN model progressively falls short of matching the data, due to the onset of direct interaction (DI) contributions and fluctuation interference effects. To allow for the DI contributions, thier magnitudes have been evaluated using coupled-equations and direct-interaction programs.

UNIVERSITIES

University of Maryland

Department of Chemistry -01 $88 K

Radioactive Decay Studies at TRISTAN II

W. B. Walters

The purpose of these studies is to determine the positions, decay branches, decay multipolarities, spins and parities of the excited levels in nuclides populated in the decay of selected fission product nuclides isolated by the on-line isotope separator TRISTAN II at the High Flux Beam Reactor at Brookhaven National Laboratory. Gamma ray singles and coincidence spectra will be measured using a multidetector coincidence and angular correlation system that is under development. Nuclides of interest span the region in which the nuclear shape is transforming from the closed shell at N=82 to deformed structures for N>90, or lie near the double magic ^{132}Sn nucleus.

UNIVERSITIES

Massachusetts Institute of Technology
Laboratory for Nuclear Science/Spectroscopy Laboratory -01 $73 K

M.S. Feld, P.G. Pappas, D.E. Murnick, M. Deutch

Laser-Induced Nuclear Orientation. Laser-induced nuclear orientation and its applications is being explored in this project. The basic idea is to use intense monochromatic laser radiation to optically pump isomeric atoms, i.e., atoms whose nuclei are in isomeric states. The nuclear orientation thus induced manifests itself in the angular distribution of the subsequent nuclear emission and decay. By employing the techniques of laser saturation spectroscopy extremely narrow resonances ($\sim 10^{-7}$ to 10^{-8}eV), comparable in resolution to Mossbauer effect resonances, should be attainable. Observation of the effect leads to determination of excited state nuclear moments and isomer shift.

Laser-induced nuclear orientation has been observed via gamma ray anisotropies in two separate systems; one, ^{22}Na, in a cell and the second, ^{24m}Na, produced on-line using a Van de Graaf accelerator. Preliminary results of the ^{24m}Na experiments have shown that the g factor is negative in ^{24m}Na and that the ^{24}Na - ^{24m}Na isomer shift is less than 240 MHz.

Efforts are under way to produce dense targets and beams with a high degree of polarization for use in nuclear physics. Experiments are on going in two atomic systems - lithium and sodium.

UNIVERSITIES

The University of Michigan
Department of Nuclear Engineering -02 $128 K

G. T. Baldwin, D. J. Grady, G. F. Knoll, M. Mahdavi, and D. McKeon

I. Absolute Fission Cross Section. We are completing a series of measurements on U-233 and Np-237 using our photoneutron source facilities. These measurements will yield absolute fission cross sections at discrete energies ranging from 23 to 964 keV. Techniques are similar to those we have employed in previous absolute cross section measurements on U-235 and Pu-239. Neutron source strengths are measured in the University of Michigan manganese bath relative to the secondary national neutron standard NBS-2.

II. Capture Cross Section Measurement Using Photoneutron Sources. Two independent experiments are currently in progress that are aimed at the determination of absolute capture cross sections. The first involves capture in In-115, and will employ $4\pi\beta$-γ detection of the induced activity in a series of target foils. This capture cross section is of primary interest as a standard in the keV neutron energy range.

We are also involved in a measurement of the Th-232 capture cross section at 23 keV. This cross section is of considerable technological interest, and will also be measured using activation techniques.

III. Facility Development for Measurement at 14 MeV. The installation of a 14 MeV neutron generator is nearing completion in a new laboratory that formerly housed the University of Michigan cyclotron. Our plan is to use these facilities for the measurement of absolute cross sections using both proton recoil monitors and associated particle counting for flux determination. We will begin with a series of fission cross section measurements on U-235, Pu-239, U-233, Np-237, and U-238. Targets used for these measurements will be the same fissile foils used for previous photoneutron experiments.

UNIVERSITIES

University of Michigan
Department of Physics -01 $55 K

Precision Positron Polarimetry--A New Technique in Weak Interaction Studies

Arthur Rich, David E. Newman

This is the first experiment to use the high precision comparison of positron polarization from different nuclei to test weak interaction beta decay theories. The basis of this technique is the use of a new type of positron polarimeter which, in conjunction with a beta spectrometer, will allow us to measure the difference in polarization of positrons from two sources to precisions two orders of magnitude better than is currently possible.

We are using this technique in an initial experiment to compare the polarization of positrons from ^{22}Na and ^{68}Ga. Previous studies of ^{22}Na decay have produced a number of mutually inconsistent experimental measurements which imply a polarization difference of up to 10^{-2} for these nuclei. We expect to achieve an accuracy of $2 - 3 \times 10^{-3}$ and thus we should be able to discriminate clearly among these predictions.

A further and probably more significant result of this work should be the successful demonstration of our polarization comparison technique as it applies to a number of tests of fundamental weak interaction theories. By selecting the nuclei to be studied, and with some modification of the apparatus, we eventually expect to search for Fierz interference and second class currents, measure weak magnetism, and contribute to the study of time reversal using this technique.

UNIVERSITIES

Middle Tennessee State University
Department of Chemistry and Physics -01 $35 K

Nuclear Structure Studies via Neutron Interactions

R. F. Carlton

This is a collaborative effort with ORNL staff at the Oak Ridge Linear Accelerator (ORELA). An analysis is underway of neutron transmission measurements made at the ORELA to systematically investigate neutron cross sections for stable isotopes relevant to tests of nuclear models. A graphics terminal will be established on campus to permit use of computer facilities at ORNL.

Initial studies will involve ^{122,124}Sn and ^{186,182,188}Os.

UNIVERSITIES

University of New Mexico
Department of Chemistry -04 $93 K (24 mos.)

The Development of Surface Immobilized Ligands for Actinide Separations

Robert T. Paine

The project is directed toward the development of improved syntheses and purification schemes for dialkyl-N,N-dialkylcarbamylmethylene phosphonate and dialkyl-N,N-dialkylcarbamyl phosphonate ligands which are currently employed in advanced actinide waste reprocessing schemes or show promise for such applications. The coordination chemistry of these ligands is being explored with transition metal, lanthanide, and actinide ions typically present in HLLW solutions. The characterization and structure elucidation of the isolated complexes by infrared, visible-UV, ESR and multinuclear NMR spectroscopies and single crystal X-ray diffraction analyses are leading to a more thorough understanding of the metal ion extraction processes. The results of this program and the presence of several practical problems in the process chemistry have led to investigations which produced routes to the chemical bonding of phosphonate ligands on silica. The program now is specifically involved in the following projects: perfecting extractive purification schemes for free phosphonates; expanding the synthetic routes for the immobilization of phosphonates on silica and other inorganic supports; characterizing the ligand bonding mode on silica using various spectroscopic techniques; examining the coordination chemistry of the bonded ligands; determining the structures of actinide ion-phosphonate complexes and determining the potential of the silica/ligand materials as single phase extraction column packing substances.

UNIVERSITIES

The University of New Mexico
Nuclear Engineering Department -02 $61 K

J. C. Robertson, D. Sloan

I. Absolute Fission Cross Sections in the 14 MeV Region. Measurements are being made of the absolute fission cross sections of U-235, Pu-239, U-233 and Np-237, in the 14 MeV energy region. In addition the angular distribution of the fission fragments is being measured as a separate project. These measurements are required because the presently available data are inadequate and not sufficiently accurate.

II. A 14 MeV Recoil Proton Monitor. A 14 MeV proton recoil monitor has been designed and constructed to measure the absolute neutron flux in the 14 MeV fission cross section measurements. Extensive calculations of the efficiency of this monitor have been made and compared with the calculations of other authors. It is clear that a major source of uncertainty in the efficiency is the lack of precise knowledge of the angular distribution of the n-p elastic scattering cross section. The efficiency can alter by up to 3% depending on the form of the angular distribution which is used.

III. K-Correction in $4\pi\beta$-γ Coincidence Counting. The magnitude of the K-correction in determining the absolute activity of foil sources by $4\pi\beta$-γ coincidence counting is being investigated as a function of Z, thickness and β end point energy. The magnitude of this correction, which allows for complex decay schemes and the counts produced in the β-counter by gamma radiation, has not been well established. This limits the accuracy which can be achieved in foil source standardization.

UNIVERSITIES

Brooklyn College of CUNY
Dynamitron Laboratory -01 $72 K

High Resolution Photofission Measurements in ^{238}U and ^{232}Th.

H. Lancman.

Previous photofission measurements have been carried out with a gamma ray energy resolution of $\sim$ 100 keV, mainly using bremsstrahlung. This resolution makes it impossible to study details of structure in the energy dependence of photofission cross sections near threshold. Our measurements employ photons from known (p,γ) resonances in a number of nuclei. This technique takes advantage of the Doppler shift of the energy of the photon emitted by the recoiling nucleus at a given proton resonance. Typical energy spreads vary between 20 and 40 keV and an energy resolution of 200 eV is easily attainable. The yield is typically 10^3 photons per μA of proton beam on target, which makes it necessary to use high beam currents. The measurements are being carried out on our 3.75 MeV Dynamitron which has a maximum proton beam current of 2 mA. Polycarbonate films are used as fission track detectors.

Our aim is to determine the photofission cross sections of ^{238}U and ^{232}Th in the 5 - 13 MeV range of excitation energy. The number of suitable (p,γ) resonances is adequate for covering this range with an average energy step of 100 keV. Regions of particular interest, especially those near threshold can be covered almost continuously. The very high gamma ray energy resolution makes it possible to search for structure in the cross section resulting from class II states in the second well of the fission barrier. The results are being compared with model calculations in order to determine the barrier parameters of the two nuclei.

UNIVERSITIES

University of Albany, New York -02 $29 K

Neutron Physics Research

J. B. Garb, V. K. Tikku (University of Albany)
J. A. Harvey, R. L. Macklin (ORNL)

Neutron Total Cross Section in the Resonance Region

These studies performed with ORELA, provide information on the parameters (E_o, Γ_n, J^π etc...) of a large number of resonances in many nuclei. From this information, one can investigate the average quantities such as nuclear level densities and strength functions, which are related respectively to nuclear structure and neutron interaction mechanisms, below 1 MeV. One can investigate the parameters of the optical model and characteristics of intermediate states. The distribution of level spacings and neutron reduced widths are also useful in the understanding of neutron-nuclear interaction processes.

Neutron Capture Cross Sections

These studies are complementary to the total cross section studies and have a greater sensitivity for the detection of weak levels which are usually populated by p- or d-wave neutron capture. Hence these studies provide additional information about the average properties of the higher angular momentum states. In addition these studies also provide values of radiative widths, which are useful in the calculation of resonance absorption integral for reactor application. Moreover the energy averaged values of neutron capture cross sections in the 30-100 keV region, in some nuclei also provide useful data for the study of nucleosynthesis of elements in astronomical applications.

UNIVERSITIES

University of North Carolina at Chapel Hill -01 $178 K

Studies of Nuclear Processes at Triangle Universities Nuclear Laboratory (TUNL)

T. B. Clegg, E. J. Ludwig, E. Merzbacher, W. J. Thompson

I. Polarization Effects in Nuclear Reactions. Beams of polarized protons and deuterons from the TUNL Lamb-shift polarized ion source are used for studies of nuclear reaction mechanisms and nuclear spectroscopy. Nuclear reactions induced by polarized deuterons have been used to investigate the mechanism by which one or more nucleons are picked up from various nuclei. The patterns exhibited by the vector and tensor analyzing powers are frequently indicative of the spin and parity of the residual levels and the angular momentum involved in populating these levels.

II. Spin-Dependent Potentials in Nuclear Scattering. Experimental and theoretical research in this area includes the following: the energy dependence of nucleon spin-orbit potentials, the relation of d,t, ^{3}He and heavy-ion spin-dependent potentials to nucleon potentials, spin-spin effective interactions in nucleon-nucleus scattering, and the effects of nuclear structure on scattering potentials.

III. High Resolution Studies of Resonances. Beams of polarized and unpolarized protons are used to excite isospin-forbidden resonances in nuclei. The TUNL high-energy-resolution system is employed since these resonances are usually narrower than the normal accelerator beam resolution. These studies are designed to attempt to establish the origin of the apparent isospin mixing. The reduced widths of these resonances are determined for a range of self-conjugate target nuclei.

IV. A New Facility for Scattering Spin-Polarized Neutrons. Spin-polarized beams of protons and deuterons have been heavily utilized tools for TUNL research programs since 1970. Often these beams have been tools to study scattering and reaction processes in which outgoing neutrons have been detected. These measurements have been severely hampered by an inability to determine accurately the outgoing neutron energy. Within the past year we have been able to pulse these polarized beams with high efficiency so the outgoing neutron energies can be accurately measured by determining their flight time from target to detector. This new facility is being exploited heavily, using the $D(\vec{d},\vec{n})^3He$ reaction to produce polarized neutrons, to measure cross sections for elastic scattering of polarized neutrons from a wide range of nuclei. The data obtained have previously been unavailable with sufficient accuracy to test theoretical methods of the spin-dependence of the neutron-nucleus interaction.

V. Atomic Effects on Nuclear Reactions. These investigations aim to explore the interface between atomic and nuclear physics by observing energy changes in nuclear systems induced by the electrons immediately surrounding the nucleus. Phenomena such as very narrow resonances in scattering from light nuclei, as observed using polarized beams and the TUNL high-energy-resolution system, are being studied.

UNIVERSITIES

North Carolina State University -01 $65 K
Triangle Universities Nuclear Laboratory -02 $70 K

C. R. Gould, G. E. Mitchell, L. W. Seagondollar, D. R. Tilley

I. High Resolution Resonance Studies.* A variety of ultra high resolution resonance experiments are being carried out on both the 3 MV accelerator and the FN tandem accelerator. Although there is still appreciable interest in global statistical properties (strength functions, average level densities), our major emphasis is on detailed or local statistical properties. These include short and long range correlations in level spacings, and unique measurements of interference effects for reduced width amplitudes. These latter results have provided the first verification of several theoretical predictions, as well as establishing new, as yet unexplained results.

II. Radiative Capture Reactions.* The main emphasis of these studies has been to search for effects of the giant quadrupole resonances in the radiative capture reaction for a variety of nuclei. Most of the E2 effects we have observed are consistent with only direct radiation which gives a "background" which makes the observation of E2 resonances difficult. Using our high intensity polarized neutron beam, we have shown that the neutron capture reaction appears to be a more favorable tool for studying E2 resonances since the direct strength is quite small. We are also using the polarized neutron beams to pursue our interest in few nucleon systems (e.g. $\vec{n}+{}^{3}He(n,\gamma)^{4}He$). These experiments are important since the few body problem is susceptible to "exact" calculations. We are continuing our use of proton beams from the Cyclo-Graaff (18-31 MeV) to study capture leading to highly excited bound and unbound final states. Our aim is to understand the reaction mechanism, to search for resonances built on these excited states, and to investigate the utility of "high energy" capture for studying highly excited states in the residual nuclei.

III. Neutron Cross-Section Studies.* Measurements of the interaction of neutron beams with a wide range of elements has been a major program at our laboratory for several years. One emphasis has been on the elastic scattering of neutron beams to permit development of more accurate nuclear models and also to provide accurate data for the design of fusion-energy sources. The second emphasis is to obtain information on the emission spectrum of secondary neutrons that are emitted when high-energy neutrons impinge on various isotopes that may comprise containment vessels or blankets for fusion-energy devices. The data is combined with theoretical models to generate better descriptions for inelastic neutron interactions. The energy of the incident neutrons in both of the above studies is 8 to 14 MeV, a region where neutron data of this type has been scarce.

*These projects are done in collaboration with faculty members from Duke University.

UNIVERSITIES

North Carolina State University
Department of Physics -01 $196 K (36 mos.)

A Cryogenic Polarized Target Facility

C. R. Gould, D. G. Haase

The identification of spin-spin effects in nucleon-nucleus scattering has been the object of continued study over the last decade. Measurements of spin-spin cross sections require that polarized beams and/or polarized targets be available. We propose to construct a cryogenic polarized nuclear target facility to be used in conjunction with the polarized neutron beam at the Triangle Universities Nuclear Laboratory to investigate spin-spin effects in nuclei which heretofore have not been easily polarizable. Recent developments in ultra-low temperature refrigeration and in superconducting magnet technology now make possible the construction of a facility for the brute force polarization of several nuclei, including ^{27}Al, ^{51}V, ^{93}Nb ^{115}In and ^{209}Bi, at millikelvin temperature in high magnetic field. In the proposed experiments cross sections will be measured for neutrons in the energy range 10 to 20 MeV. Both transverse-spin and parallel-spin geometries will be used in order to study the central and tensor contriburions to the spin-spin force. These experiments will be useful not only for the nuclear physics information acquired but also in demonstrating the feasibility and usefulness of brute force polarization and outlining its further applications.

UNIVERSITIES

Ohio University
Accelerator Laboratory -02 $167 K

R.O. Lane

I. Structure of Light Nuclei. The special features of the Ohio University tandem accelerator are employed to probe the light nuclei via neutron elastic and inelastic scattering to yield structure information for the development of models for these nuclei. For many of the light nuclei charged particle and γ-ray reactions so common in the past have reached a limit in definitive new nuclear structure contributions, whereas the long overlooked neutron reactions when properly pursued with this unique facility are now contributing to further development of shell models and cluster models of the light nuclei. The data obtained in these studies are in most cases directly applicable to the fusion energy program by way of cross sections needed for shielding purposes as well as cross sections and nuclear model development to better predict tritium breeding and other reactions taking place in future fusion energy devices.

II. Neutron-Induced Reactions. Again the special features of this accelerator are exploited study charged particles emerging from neutron bombardment of nuclei. A truly unique spectrometer for this use has been designed and constructed at this laboratory. Virtually no measurements of these properties exist over an energy range needed both to study the nuclear reaction mechanism and to provide vital data to designers of fusion energy reactors of the future. Present-day fusion energy concepts involve reactions which produce copious quantities of neutrons which in turn can cause internal damage to structural members by the charged particles produced inside them by the high neutron flux. Theoretical studies of the data will provide an interpretation method and model development for extension to other nuclei where data do not exist.

III. Analytical Theory Development. In order to compare these measurements to the predictions of fundamental compound nuclear models it is usually necessary to analyze the data by means of an intermediate or analytical theory which interprets the data in terms directly comparable to fundamental models. New developments in this rather complex analytical theory are being made to encourage greater interaction between theory and experiment and, therefore, greater progress in our fundamental understanding of the nucleus.

UNIVERSITIES

University of Oklahoma
Department of Physics and Astronomy -01 $55 K (22 mos.)

Spectroscopic Studies of Transitional Nuclei

R. F. Petry

Studies of the levels in neutron-rich ^{90,92}Kr and ^{140,142}Xe populated in the beta decay of ^{90,92}Br and ^{140,142}I are underway at the TRISTAN II facility at Brookhaven National Laboratory. The objectives of the measurements is the characterization of the transition from sperical to deformed shapes in the medium-mass region. Of particular theoretical interest are now shell-model calculations of the shape transition in the A~100 region, and the Interacting Boson Model calculations on SU(5)→SU(3) transitions.

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UNIVERSITIES

University of Pennsylvania
Department of Physics -03 $79 K

Compilation of Information on the Energy Levels of the Light Nuclei
FY 1978 $77,507

F. Ajzenberg-Selove

This work consists of two parts. The first is the review and avaluation of all the information available about the nuclei with $5 \leq A \leq 20$, where A is the total number of neutrons and protons in the nucleus. On the average, there are some 1500 new publications/year worldwide on these light nuclei. We evaluate these publications in the light of all other knowledge on these nuclei and prepare definitive summaries which are published once a year by the journal Nuclear Physics, generally as a complete issue of that journal. Each summary evaluates the work on two to five A-chains (families), the exact number depending on the complexity of the information. These evaluations are used throughout the world not only by basic nuclear scientists but also by scientists concerned with applications to the CTR program, nuclear medicine, etc. In 1979 we published "Energy Levels of Light Nuclei, A = 5-10" in Nuclear Physics A320 1-224 (1979).

The second part of our work consists in collaborative, user-type research at P-9 at Los Alamos using 17-25 MeV tritons and the very high resolution Q3D spectrometer equipped with a helical proportional chamber. This past year we have been studying the (t,p) reactions on the Molybdenum isotopes. The studies of these two-nucleon transfer reactions are being used, inter alia, to understand the change in the structure of the Mo isotopes as one goes from the low A isotopes of that element to the high A isotopes.

While the evaluation work is more immediately relevant, our work at Los Alamos which is done with frontier-type equipment and analysis methods makes us able to better evaluate contemporary research papers.

UNIVERSITIES

Princeton University -01 $165 K

Nuclear Chemistry Project

R.A. Naumann, K. Krien, F. Girshick, F. Loeser

I. Charged Particle Nuclear Spectroscopy. These experiments involve the selective (p,t) and (t,p) two nucleon transfer reactions and high resolution Q3D spectrographs to study characteristics of the levels in medium and heavy nuclei. Investigations involving radioactive nuclei are included in this program. When applied to nuclei with an uneven number of protons and/or neutrons these transfer reactions preferentially populate those levels of the product nucleus having a configuration of the unpaired nucleon(s) related to that of the target nucleus. Comparisons of the spectra obtained for adjacent nuclei thus test the extent to which collective and single particle properties of nuclei are preserved on the addition of one or two nucleons.

II. In-Beam Studies of Nuclear Excited States. Nuclear reactions involving charged projectiles and subsequent neutron evaporation provide a general means for preparing excited states of nuclei in a state of polarization. However, studies of the gamma rays accompanying deexcitation of these states often fail to reveal the decay of nuclear isomeric states where low energy transitions and/or long lifetimes are involved. Since such isomeric transitions proceed predominantly by the emission of conversion electrons, an on-line magnetic electron spectrometer has been recently installed at the Princeton Cyclotron for their study. This instrument is being used to study the lifetimes, gamma ray multipolarities and moments of nuclear isomeric states by direct observation of the conversion electrons accompanying nuclear reaction.

III. Atomic Coulomb Capture of Negative Muons (in collaboration with Dr. J. D. Knight, Los Alamos). When negative particles slow in an absorber they decelerate and are captured in the positive electric field of a nucleus by energy loss to the bound atomic electrons of the absorber. After this initial binding, the negative particle passes to more deeply bound orbits by further energy loss involving electron ionization (Auger process) or radiation. A weakly interacting particle reaches the lowest bound atomic 1s state, signalling its arrival by emission of characteristic X rays. At the LAMPF meson facility employing muon beams, we measure the relative intensities of emitted muonic X rays to investigate the marked dependence of this capture process on the physical and chemical state of the atoms comprising the absorber.

UNIVERSITIES

Rensselaer Polytechnic Institute
Department of Nuclear Engineering -02 —($134 K/24 mos.)

Fission Cross Section Measurements of the Even Curium Isotopes

Robert C. Block

The neutron-induced fission cross sections of $^{244,246,248}Cm$ will be measured from approximately 1 eV to 100 keV using a 75-ton lead slowing-down spectrometer. The intense neutron flux provided by the spectrometer enables the neutron-induced fission to compete with the spontaneous fission background and also permits the use of microgram quantities of highly enriched curium samples.

UNIVERSITIES

University of Tennessee
Department of Physics -04 $65 K

Magnetic Measurements of the Transuranium Elements and Charge State Characterization of Actinides in Monazite

Paul G. Huray

The program has both an applied and a basic research thrust through investigations of the physical properties of the transuranium elements and their compounds. Because of the natural α-decay of the elements Pu, Am, Cm, Bk, Cf, and Es the research is carried out at the Transuranium Research Laboratory of the Oak Ridge National Laboratory. Macroscopic quantities (greater than one microgram) of these elements are periodically milked from the High Flux Isotope Reactor, purified, and prepared as oxides and various crystallographic forms of the metal. With our (S.Q.U.I.D. based) micro-magnetic susceptometer we are examining the effective high temperature magnetic moments and low temperature magnetic transitions in order to determine the effective number of 5f electrons per atom and the magnitude of their overlap in the compounds and metals. With our Mössbauer apparatus we are examining the charge state of Np ions as impurities in $LaPO_4$ crystals. This compound (synthetic Monazite) shows strong resistance to leaching of the radioactive impurity for most transuranium elements and has therefore been proposed as a primary containment form for actinide wastes. Our charge characterization will likely aid the interpretation of the strong chemical bonding mechanism which produces this feature of the compound.

UNIVERSITIES

University of Tennessee
Department of Chemistry -04 $100 K

Physical-Chemical Studies of the Transuranium Elements

Joseph R. Peterson

The program provides training for pre- and postdoctoral students in chemical research with the transuranium elements through continuing investigations of the basic physical-chemical properties of these elements and the interpretation and correlation of the results obtained. New knowledge is expected to be accumulated in the role of the 5f electrons in bonding in actinide elements and compounds, the relationships of metallic structures to metallic valence and radius, the extent and magnitude of the actinide contraction, the magnetic, thermodynamic, spectroscopic, and crystallographic properties of these materials as related to general theories, the effect of self-irradiation on chemical and physical properties, the chemical consequences of radioactive decay, and in general, the range of validity of the actinide hypothesis. Specific projects include: synthesis of Cm-248, Bk-249, and Cf-249 metals for X-ray diffraction (vary temperature or pressure), magnetic susceptibility (SQUID-based microsusceptometer), and heat of solution (solution microcalorimeter) studies; spectral and X-ray diffraction studies of mixed-valence lanthanide, actinide, and mixed lanthanide-actinide halide compounds, transamericium element fluorides, and halide compounds resulting from the radioactive decay series $^{253}Es \rightarrow {}^{249}Bk \rightarrow {}^{249}Cf$; study of the chemical consequences of radioactive decay in the bulk phase solid state; spectroelectrochemical studies of actinides to characterize unusual oxidation states such as Am(VII), Cm (V), Bk(II), Cf(V), and Es(IV); growth of crystals of transamericium element phosphates for optical and structural characterization over time to study the effects of self-irradiation on the chemical and physical properties of these synthetic monazites.

UNIVERSITIES

Tennessee Technological University
Chemistry Department -04 $102 K (24 mos.)

The Investigation of the Solution Properties of the Transuranium Elements

Dale D. Ensor

The emphasis of this program is to investigate the basic properties of the transuranium elements in aqueous solution. Information gained in these investigations would be applicable to the improvement of separation techniques for the actinide elements from one another and from the chemically similar lanthanide elements. Major effort will be devoted to the evaluation of novel macrocyclic compounds as solvent extraction agents for the trivalent actinides. The size selective nature of these compounds as exhibited by their behavior with the alkali metal could allow separations based on cation size. Investigations to better define the complexation reactions of the transuranium elements by measuring the appropriate thermodynamic properties (Δ G, Δ S, Δ H) are currently underway. The measurements are concentrated on the aminopolycarboxylate complexes which are important in certain separation schemes now used. The information obtained will be useful in better defining the role of the 5f orbitals in complexation reactions of the transuranium elements.

UNIVERSITIES

Texas A&M University
Department of Physics
Stored Ion and Laser Physics Laboratory -01 $95 K (24 mos.)

Hyperfine Structure and Isotope Shift Measurements of Short-Lived Elements by Laser Spectroscopy

H. A. Schuessler and H. S. Lakkaraju

Novel experimental studies of nuclear moments and charge distributions for short-lived isotopes far from the valley of nuclear stability are initiated. The basic difficulty in the experiments is due to the small number of radioactive nuclei available even with modern on-line mass separators and due to the finite lifetime of these nuclei. Two sensitive methods are being developed. One uses radioactive ions stored electrodynamically for considerable periods of time in a radio-frequency quadrupole ion trap. The other employs intracavity Doppler-free fluorescence spectroscopy. In the ion storage method, as few as a thousand ions can be investigated. The ions are stored in ultrahigh vacuum during their lifetime and practically float in free space. Laser excitation of stored radioactive ions will be used to measure the hyperfine structure splitting and eventually to cool the ions by optical sideband excitation to a temperature of less than $1^{o}K$. The high sensitivity and speed of intracavity fluorescence measurements will be utilized in the second experiment. After the present initial phase of the experiments where the unknown hyperfine structure of stable isotopes is investigated, the experiment will in the second phase be moved to the on-line mass separator at Brookhaven and should yield information on nuclear charge distributions, nuclear moments and spins in new mass regions.

UNIVERSITIES

Texas A&M University
Cyclotron Institute -01 $84 K

Contribution to Costs of Beam Time for Nuclear Science Research

D. H. Youngblood

The Texas A&M 88" cyclotron provides proton ($\leq$55 MeV), deuteron ($\leq$65 MeV), ^{3}He ($\leq$130 MeV) and α particle ($\leq$130 MeV) beams as well as a variety of heavy-ion beams for nuclear science research. Polarized proton, deuteron and ^{3}He beams are also available for experiments. Projects under way at the laboratory include the following. The multipole strength distribution in nuclei is being investigated with emphasis on the properties of the isoscalar giant monopole resonance. These studies are done with inelastic scattering of 130 MeV alpha particles at small angles where the monopole is enhanced. Tests of the isobaric mass multiplet equation made by measuring the masses of both proton-rich and neutron-rich nuclei are in progress. Parity violation in the hadronic weak interaction is being explored by asymmetry measurements of elastically scattered longitudinally polarized protons at 50 MeV on a hydrogen target. Studies of few nucleon systems are under way with emphasis on measuring spin correlation nucleon-nucleon parameters.

UNIVERSITIES

University of Washington
Nuclear Physics Laboratory -01 $755 K

E.G. Adelberger, J.S. Blair, D. Bodansky, J.G. Cramer, G.W. Farwell, I. Halpern, F.H. Schmidt, K.A. Snover, T.A. Trainor, R. Vandenbosch, W.G. Weitkamp

I. Nuclear Astrophysics. These studies are to obtain nuclear data needed for a detailed description of nucleosynthesis in astronomical environments and of the processes by which energy is generated in these environments. Such data is necessary both for the formulation of quantitative models, and for the testing of hypotheses as to the character of the physical processes involved.

II. Fundamental Symmetries. Those aspects of the fundamental interactions which can best be investigated through experiments on nuclear or atomic systems are studied; particularly those cases where the nuclear or atomic physics is exceptionally simple and well understood, so as best to illuminate the basic symmetries unencumbered by uncertainties in the many-body problem. Topics of current interest include parity mixing in light nuclei and hydrogenic atoms, β decay, and the detailed study of the breakdown of isospin symmetry. A more sensitive test of nucleon charge conservation has been performed.

III. Radiative Capture Reactions. This research program places major emphasis on the study of magnetic dipole and electric quadrupole strength. Our purpose is to deduce through detailed studies of particular nuclei the strength distribution of magnetic dipole and electric quadrupole radiation produced in radiative capture. These measurements enable the characterization of the strength distribution not only to nuclear ground states but to excited states as well. The study of strength distributions for excited states is a new development with a large potential range of applicability.

IV. Polarization Effects in Nuclear Reactions. We are carrying out a number of experiments which exploit the Lamb-shift polarized ion source as a probe of nuclear reaction mechanisms. Determination of the depolarization parameter and very accurate measurements of the analyzing power for particle emission to highly excited residual nuclei are directed toward understanding the continuous variation of reaction mechanisms from one-step excitation of single levels to absorption of a projectile with later evaporation of another. Additional analyzing-power measurements which emphasize elastic scattering and inelastic scattering to discrete levels in the residual nucleus complement the above program.

V. Accelerator Radiochronology. This newly-developed approach to radiometric dating will enable measurement of minute isotopic fractions using small amounts of source material. Present emphasis is on the development of precise techniques for the measurement of $^{10}Be/^{9}Be$ and $^{14}C/^{12}C$ ratios.

UNIVERSITIES

UNIVERSITY OF WASHINGTON
Department of Nuclear Engineering -02 $30 K

Neutronics Research

G.L. Woodruff, P.J. Grant, D.L. Johnson

I. Delayed Neutron Spectroscopy. This work has consentrated on the measurement of near-equilibrium neutron energy spectra from fertile and fissile nuclei. The results are significant in the area of reactor safety, nuclear safeguards, and the level structure of nuclides far from the line of nuclear stability.

II. Alpha-n Yields. These experiments are devoted to accurate measurements of the neutron yields from (α,n) reactions in low Z nuclides relevant to reactor applications. Particular emphasis is placed on results from higher alpha energies than used in previous experiments. The results will be important for subcritical reactivity monitoring, nuclear safeguards, and shielding requirements for both reprocessing and nuclear waste storage.

UNIVERSITIES

University of Wisconsin
Nuclear Physics Laboratory -01 $55 K

L.D. Knutson and P.A. Quin

I. Charge Symmetry in Neutron-Proton Scattering: Nuclear forces are said to obey the principle of charge symmetry if the interactions are invariant under the interchange of neutrons and protons. This symmetry principle apparently holds in nuclei (no firm evidence for violation of charge symmetry has been found) provided that one corrects for the effects of electromagnetic interactions. An experiment is being undertaken which will allow us to test the principle of charge symmetry in the neutron-proton system by measuring the analyzing powers for the scattering of polarized neutrons by unpolarized protons and for the scattering of unpolarized neutrons by polarized protons. If charge symmetry holds, the two analyzing powers will be equal. This experiment differs from previous tests of charge symmetry in that the interpretation of the results will be free of complications caused by electromagnetic interactions. The experiment will be carried out at the Indiana University Cyclotron Facility at a neutron energy of 200 MeV. A major part of the project involves the development and construction of various pieces of experimental apparatus including a liquid deuterium target for the production of polarized neutrons, a polarized proton target which makes use of the "spin refrigerator" method for producing polarized protons, and a pair of high-efficiency, position-sensitive neutron detectors.

UNIVERSITIES

University of Wisconsin
Nuclear Physics Laboratory -01 $615 K

W. Haeberli, L.D. Knutson, D. Mavis, P. Quin, H.T. Richards, S. Sen

I. Fundamental Symmetries: An experiment to test whether scattering of longitudinally polarized protons by protons exhibits mirror symmetry (i.e. parity conservation) is near completion. The results thus far indicate a non-zero longitudinal analyzing power of $(-3.2\pm1.1) \times 10^{-7}$. If mirror symmetry holds this quantity should be zero.

II. Radiative Capture of Polarized Particles: Our intense source of polarized protons and deuterons offers an unique opportunity to explore radiative capture of polarized neutrons. These experiments will concentrate on isospin effects in the giant dipole resonance (GDR) of light nuclei. The relatively neglected $(\vec{d},\gamma)$ reactions have also become feasible and may help to understand the role of isospin mixing in the GDR, especially for self-conjugate nuclei. A large NaI spectrometer is under construction for these studies.

III. Direct Reactions with Polarized Deuterons: Measurements of the vector analyzing power are being used to obtain spectroscopic information for a number of nuclei. Tensor analyzing power measurements allow one to probe the D-state components of the deuteron and triton wave functions.

IV. Nucleon-Nucleon Experiments: Experiments to study the spin dependence of the fundamental nuclear interaction by measuring the analyzing powers for nucleon-nucleon scattering are in progress. The analyzing power is being measured for p-p scattering at 10 MeV and for n-p scattering at 25 MeV. In another experiment, the reaction $\vec{n}+p \rightarrow d+\gamma$ is being studied as a potential new source of information about the nucleon-nucleon interaction.

V. Cluster States from Alpha Scattering and Reactions. Resonant scattering and reactions of alphas on light alpha particle nuclei yield precise information (J^{π}, E_R, Γ, Γ_R/Γ) of many highly excited cluster states.

VI. Ion Source Research and Development: Our proposal for the development of intense sources of polarized alkali beams by optical pumping with dye lasers is under investigation. Development work on the colliding beam polarized ion source and on the cesium sputter source for heavy metal ions continues.

UNIVERSITIES

Yale University
A.W. Wright Nuclear Structure Laboratory -01 $285 K

D.A. Bromley, P.D. Parker, et al.

I. Nuclear Science with Light Ions. Having discovered pairing isomers -- a new form of nuclear excitation probing deeply buried nucleon orbitals -- in our studies of the tungsten isotopes we are scanning a much wider range of targets to establish the systematics of these isomers and thus a new aspect of nuclear shell structure; many new examples have been identified. We have completed our determination of the matrix elements for the nucleon-nucleon residual interaction in the lead region; for the first time it has been possible to study a number of the valence shells and in addition to measuring the T = 1 matrix elements for the first time we have demonstrated the importance of explicit core polarization phenomena. From inelastic alpha particle studies on very highly excited, high spin states in light nuclei we have extended our spectroscopic studies to very high members of rotational bands based on simple shell configurations. And continuing our work in nuclear astrophysics we have made extensive new measurements on the mass 37 system and on the radiative capture of alpha particles by helions, both critical to our understanding of solar neutrino astronomy.

II. Nuclear Physics Applied to Other Sciences. We have continued to apply our hydrogen profiling technique to many other sciences. Work on the development of a much improved bottle for storage of ultra cold neutrons continues as does work on the detailed mechanisms for hydrogen migration in metals and other solids. Using our accelerator as an ultra mass separator for ^{10}Be and ^{26}Al in geochronology studies, we have established the growth rate for ocean floor manganese nodules as 4.5 mm per million years and are now studying Pacific abyssal cores to provide a detailed measurement of cosmic radiation variability over the past few million years. We have demonstrated that currently cosmic radiations (primarily muons) are a significant cause of soft failure of large computer systems and that at the next level of circuit integration they will be the dominant cause. We have developed new theories of ion induced sputtering and made measurements to distinguish between the "thermal-spike" and "ion-explosion" variants; both these and the above hydrogen migration studies are relevant to fusion reactor inner wall problems.

UNIVERSITIES

Yale University
Electron Accelerator Laboratory -01 $175 K

F. W. K. Firk

Neutron Polarization Studies

A. The Double-Scattering of Fast Neutrons by Light Nuclei.

We have continued to exploit the unique source of highly polarized neutrons available at the Yale University Electron LINAC at energies between 50 keV and 5 MeV, obtained by the elastic scattering of an intense pulsed beam of photo-neutrons from selected light nuclei. Our measurements of the absolute polarization of neutrons scattered from nuclei ranging from ^{4}He to ^{32}S, have been included in global analyses to give new information on the nuclear structure of the compound systems. For example, our results have played a key part in the discovery of a p-wave triplet of states in the important reaction n + ^{6}Li at an excitation energy below 10 MeV.

B. Polarization Effects in the Small-Angle Scattering of Neutrons:

Mott-Schwinger Scattering and the Polarizability of the Neutron.

We have studied $\vec{n}$ - ^{209}Bi elastic scattering as a continuous function of energy in the MeV region at angles between 3° and 20° with an absolutely calibrated source. Detailed calculations, using Hogan and Seyler's method of analysis, have been carried out and compared with our results. The sensitivity of the measurements, and of the analyses, to different values of the neutron polarizability coefficient has been investigated. As a consequence of this work, which involves a fundamental structure constant of the neutron, we have started a series of measurements of the polarization of low-energy neutrons scattered at small angles from nuclei in which the nuclear scattering amplitudes can be calculated exactly from a knowledge of the s- and p-wave resonance parameters. We fully expect to be able to set a significantly improved limit on the magnitude of the electric polarizability coefficient of the neutron as a result of our new studies.

OTHER

National Bureau of Standards
Nuclear Radiation Division -02 $475 K

Differential Neutron Nuclear Data Standards

C. D. Bowman, A. D. Carlson, G. P. Lamaze, M. M. Meier, R. A. Schrack, K. C. Duvall, O. A. Wasson, R. B. Schwartz, R. G. Johnson, I. G. Schröder

I. MeV Neutron Standards. These studies are aimed at improving the accuracy of cross section and flux monitors used as standards for neutrons in the MeV range. Redundancy in measurement methods is emphasized through parallel measurements using the NBS 100 MeV linac as a white source and the NBS positive ion accelerator for accurate measurements near 14 MeV. This work is aimed at improving the accuracy of MeV nuclear data needed in fusion reactor development, national defense, cancer therapy using neutrons, and performance evaluation of accelerator breeder concepts.

II. KeV Neutron Standards. These measurements are intended to increase the accuracy of reaction cross section standards in the keV range and bear on the improvement of breeder reactor concepts and on problems in national defense. Redundant measurement methods including filtered beams at the NBS reactor, monoenergetic neutrons at the ion accelerator, and white neutrons from the linac all are being used concurrently.

III. 1/v Neutron Standards. In the eV range of neutron interactions the near 1/v behavior of the neutron reaction cross sections of ^{3}He, ^{6}Li, and ^{10}B are useful neutron cross section standards. This effort is aimed at measuring the deviation from the 1/v cross section arising from both nuclear and atomic effects. These results should lead to improvements in commercial power reactor performance including several parts of the fuel cycle.

IV. Physics of Neutron Interactions With Matter. These studies are concentrated on the interaction between atomic and nuclear phenomena in the energy range above thermal neutron energies. While the emphasis is on fundamental physics, the work is expected to have application in improved understanding of neutron exposure to personnel, in development of special materials important to new technology, and might lead to some degree of control over nuclear reaction rates.

V. Neutron Source and Instrumentation Development. Improvements in neutron measurements are being pushed on two fronts: the development of better neutron sources and the development of new neutron detectors. Source development is aimed at a possible new source for the NBS and at the development of a small but intense neutron source which would allow the transfer of neutron measurement methods from the large accelerator and reactor of the laboratory to more general application in industry. New neutron detectors are aimed at improved accuracy in measurement of high energy neutrons and at better resolution and broader uses for position-sensitive neutron detectors.

OTHER

Rockwell International
Energy Systems Group -02 $70 K

Helium Production Cross Sections

Harry Farrar IV, D. W. Kneff, B. M. Oliver, M. M. Nakata

Helium Production Cross Sections for Fusion Energy Neutrons. The objective of this program is to measure experimentally the total helium generation cross sections of several separated isotopes and their associated pure elements for fusion-energy neutrons. This information is of prime importance in the development of both fusion and fast reactors because of the effects that internally-generated helium has on the mechanical and physical properties of the reactor components.

Numerous small samples are irradiated together using high-intensity neutron sources presently employed for materials testing for the U.S. magnetic fusion energy program. The helium generated in the samples is measured accurately (~1-2%) using a high-sensitivity gas mass spectrometer system. The measurements provide a direct method of determining the total helium generated by all contributing reaction channels. The helium generation cross sections are then determined from the helium measurements and the total neutron fluence received.

A significant fraction of the program effort is directed towards determining the exact spatial dependence of the neutron fluence in the irradiation assembly, since steep fluence gradients make the fluence the principal source of uncertainty in the final cross sections. This determination involves using foil activation and helium accumulation neutron dosimetry to generate a three-dimensional fluence map for the assembly. The helium accumulation neutron dosimetry uses the same helium-measuring capability of the mass spectrometer as used for the cross section determinations.

Two separate irradiations with 14.8-MeV (average energy) neutrons from a T(d,n) fusion neutron source have been completed, and helium generation cross sections for Al, Ti, Cr, Fe, Ni, ^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, ^{64}Ni, Cu, ^{63}Cu, ^{65}Cu, and Au have been determined. Additional elements, including Be, O, F, Si, V, Cr, Mn, Zr, Nb, Mo, Sn, W, Pb, and many of their separated isotopes, have been or will be irradiated, and their cross sections will be determined. Other neutron spectra will also be used, and the cross section results will be compared with available theoretical calculations to provide important experimental tie-points to check nuclear model codes and refine model parameters.

40-574 O - 85 - 21

OTHER

SRI International
Materials Research Laboratory -04 $83 K

Chemistry of the Gaseous Lower Halides of Uranium

D. L. Hildenbrand

The objective of this program is to provide an accurate thermochemical characterization of the gaseous lower-valent halides and the oxyhalides of uranium. Thermochemical data are derived largely from high temperature equilibrium measurements monitored by mass spectrometry and by the torsion-effusion method. Various types of chemical beam sources are used to generate the gaseous uranium halide and oxyhalide species of interest. Reaction enthalpies, bond dissociation energies, and standard enthalpies of formation are the primary results derived from the equilibrium studies. In addition, special emphasis is placed on deriving entropy data as well, so that the estimated assignments of spectroscopic and molecular constants of the gaseous uranium compounds can be verified. The aim is to provide sufficient information so that the energetics of reactions involving uranium halides and the equilibrium properties of these systems can be accurately evaluated over wide temperature ranges. A secondary goal is the correlation of the results with the nature of the chemical bonding in these compounds.

INDEX OF INVESTIGATORS

Adelberger, E. G., 71
Ahmad, I., 3
Ajzenberg-Selove, F., 63
Alburger, D. E., 7
Alsmiller, R. G., 25, 27
Arthur, E. D., 19

Back, B. B., 3
Baldwin, G. T., 51
Barschall, H. H., 17
Beghian, L. E., 48
Begun, G. M., 30
Beitz, J. V., 5
Bell, W. A., 31
Bertrand, F. E., 22
Betts, R. R., 3
Bhat, M., 9
Bigelow, J. E., 33
Bilpuch, E. G., 41
Blair, J. S., 71
Block, R. C., 65
Bodansky, D., 71
Borg, R. J., 17
Bowman, C. D., 77
Brenner, D. S., 36
Britt, H., 18
Bromley, D. A., 75
Brown, R., 18

Carlson, A. D., 77
Carlton, R. F., 53
Carnall, W. T., 5
Casten, R. F., 6
Cecil, F. E., 38
Cerny, J., 11
Chasman, R. R., 3
Chattin, F. R., 33
Choppin, G. R., 42
Chrien, R. E., 6
Chu, Y. Y., 8
Clark, D. D., 39
Clegg, T. B., 58
Collins, E. D., 33
Conzett, H. E., 11
Couchell, G. P., 48
Cox, J. A.,32
Cramer, J. G., 71
Cremers, T. L., 21
Cumming, J. B., 8

Dabbs, J. W. T., 24
Dairiki, J. M., 15
Davids, C. N., 2
Deutch, M., 50
Dodder, D. C., 19
Drake, D., 18
Dunford, C., 9
Duvall, K. C., 77

Edelstein, N., 16
Egan, J. J., 48
Eller, P. G., 21
Elwyn, A. J., 2
Ensor, D. D., 68
Evans, A. E., 20

Farrar, H. IV, 78
Farwell, G. W., 71
Feld, M. S., 50
Fink, F. W. K., 76
Friedman, A. M., 3
Fu, C. Y., 26

Gabbard, F., 46
Gabriel, T. A., 27
Garg, J. B., 57
Garrett, W. R., 28
Garvey, G. T., 2
Gill, R. G., 6
Gilmore, J., 18
Gindler, J. E., 3, 4
Girshick, F., 64
Glendenin, L. E., 3, 4
Goldhaber, G. S., 39
Gould, C. R., 59, 60
Goulding, F. S., 14
Gowdy, G., 6
Grady, D. J., 51
Grant, P. J., 72
Grimes, S. M., 17
Gruhn, C. R., 14
Gwinn, H. R., 31

Index of Investigators

Haase, D. G., 60
Haeberli, W., 74
Hahn, R. L., 30
Haight, R. C., 17
Haire, R. G., 30
Hale, G. M., 19
Halperin, J., 30
Halpern, I., 71
Harvey, B. G., 13
Harvey, J. A., 23, 24, 25, 57
Haustein, P. E., 8
Heath, R. L., 10
Henderson, D., 4
Henning, W. F., 2
Henry, E. A., 17
Hershberger, R. L., 46
Hessler, J. P., 5
Hildenbrand, D. L., 79
Hill, J. C., 1
Holland, R. E., 2
Holt, R. J., 2
Horen, D. J., 23
Huray, P. G., 66
Hurst, G. S., 28

Jackson, H. E. Jr., 2
Jarmie, N., 18
Johnson, C. H., 23, 24
Johnson, D. L., 72
Johnson, R. G., 77

Kane, W. R., 6
Katcoff, S., 8
Kegel, G. H. R., 48
King, L. J., 33
Kneff, D. W., 78
Knoll, G. F., 51
Knutson, L. D., 73, 74
Kramer, S. D., 28
Kraushaar, J. J., 37
Krien, K., 64
Krohn, V. E., 2
Kunz, P. D., 37
Kutschera, W., 2

Lakkaraju, H. S., 69
Lamaze, G. P., 77
Lancman, H., 56
Lane, R. O., 61
Larson, D. C., 26
Leich, D. A., 17
Lewis, D. A., 45
Lewis, T. A., 25
Lind, D. A., 37
Lindner, M., 17
Liou, H. I., 6
Lloyd, M. H., 33
Loeser, F., 64
Ludwig, E. J., 58

Macklin, R. L., 23, 57
Madland, D. G., 19
Mahdavi, M., 51
Martin, M. J., 29
Mavis, D., 74
Maya, L., 30
McKeon, D., 51
McKeon, R. D., 2
Meier, M. M., 77
Merzbacher, E., 58
Meyer, R. A.,17
Meyer-Schutzmeister, L., 2
Mitchell, G. E., 59
Mittler, A., 48
Monohan, J. E., 2
Mooring, F. P., 2
Moretto, L. G., 12
Morss, L., 5
Murnick, D. E., 50

Nakata, M. M., 78
Naumann, R. A., 64
Newman, D. E., 52
Newman, E., 31
Norbeck, E., 44

Ohlsen, G., 18
O'Kelly, G. D., 30
Oliver, B. M., 78
Ottinger, C. L., 34

Paine, R. T., 54
Pappas, P. G., 50
Parker, P. D., 75
Pearlstein, S., 9
Peelle, R. W., 25
Penneman, R. A., 21
Peterson, J. R., 67
Peterson, R. J., 37
Petry, R. F., 62
Pullen, D. J., 48

Quin, P. A., 73, 74

Index of Investigators

Raman, S., 23, 24
Reeder, P. L., 35
Reich, C. W., 10
Rich, A., 52
Richards, H. T., 74

Ringo, G. R., 2
Ristinen, R. A., 37
Roberson, N. R., 41
Robertson, J. C., 55
Rost, E. S., 37
Russell, G., 18

Schier, W. A., 48
Schiffer, J. P., 2
Schmidt, F. H., 71
Schrack, R. A., 77
Schroeder, I. G., 77
Schuessler, H. A., 69
Schwartz, R. B., 77
Seagondollar, L. W., 59
Sen, S., 74
Sheldon, E., 48
Shmid, M., 6
Slaughter, G. G., 23
Sloan, D., 55
Smither, R. K., 2
Smythe, W. R., 37
Snover, K. A., 71
Spencer, R. R., 26
Stelts, M. L., 6
Struble, G. L., 17
Sullivan, J. C., 5

Tikku, V. K., 57
Tilley, D. R., 59
Todd, H. A., 25
Tracy, J. G., 31
Trainor, T. A., 71

Vandenbosch, R., 71

Wagner, F. Jr., 5
Walter, R. L., 41
Walters, W. B., 49
Warburton, E. K., 7
Ward, J. W., 21
Warner, D. D., 6
Warner, R. A., 35
Wasson, O. A., 77
Weitkamp, W. G., 71
Weller, H. R., 41
Wester, D. W., 5
Weston, L. W., 24
Wilhelmy, J., 18
Wilkins, B. D., 3
Williams, M. L., 24
Winters, R. R., 40
Wohn, F. K., 1
Wolf, K. L., 3
Wood, J. L., 43
Woodruff, G. L., 72

Yates, S. W., 47
Yntema, J. L., 2
Young, P. G., 19
Youngblood, D. H., 70

Zafiratos, C. D., 37
Zaidins, C. S., 37

INDEX BY BUDGET CATEGORY

KC010101 LOW ENERGY NUCLEAR RESEARCH

Experimental research in low-energy nuclear physics. (Excludes research performed at accelerators capable of producing mesons, or with beams of particles heavier than the alpha particle, which is included in separate categories in the program of the Office of High Energy and Nuclear Physics.)

1, 2, 3, 6, 7, 8, 10, 11, 12, 13, 14, 17, 18, 20, 22, 23, 36, 37, 39, 41, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 58, 59, 60, 62, 64, 69, 70, 71, 73, 74, 75, 76

KC010102 NUCLEAR DATA MEASUREMENTS

Measurement programs to provide nuclear data information needed by energy and environmental technologies.

4, 10, 17, 18, 24, 25, 26, 27, 28, 35, 38, 40, 41, 48, 51, 55, 57, 59, 61, 65, 72, 77, 78

KC010103 NUCLEAR DATA COMPILATION AND EVALUATION

Includes support of the national network of nuclear structure and decay data centers as well as a major portion of the support of the National Nuclear Data Center.

9, 10, 15, 19, 29, 63

KC010104 HEAVY ELEMENT CHEMISTRY

Experimental research on the chemical and physical properties of the heavy elements (Z>83).

5, 16, 21, 30, 42, 54, 66, 67, 68, 79

KC010201 ELECTROMAGNETIC ISOTOPE SEPARATION

Subsidy of the ORNL Calutron facility.

31

KC010202 SPECIAL ISOTOPE PREPARATION

Isotope production at the High Flux Isotope Reactor, separations at the Transuranium Processing Plant, and preparation of nuclear materials for use in research; all at ORNL

32, 33, 34

1.0 Heavy Ion Fusion Accelerator Research (HIFAR)

16. What level of funding for each of FY 1984 - FY 1986 was assumed by the revised multi-year plan for the Heavy Ion Fusion Accelerator Research (HIFAR) for the first-stage plan? How do these compare with the estimated funding levels for FY 1984 and FY 1985?

Answer: The multi-year plan for Heavy Ion Fusion Accelerator Research (HIFAR) program was developed in 1982-83 and published in May 1983 (Los Alamos National Laboratory LA-UR-83-1717). In FY 1984 dollars funding proposed for Stage I (FY 1984 - FY 1986) is as follows: $5.0 M in FY 1984; $11.0 M in FY 1985; and $17.0 M in FY 1986, for a total of $33.0 M. For comparison, the actual appropriation in FY 1984 is $5.0 M; and the President's Budget request for FY 1985 is $9.0 M.

17. What is the impact of the reduced funding levels for FY 1984 and FY 1985 on the Phase I HIFAR program schedule? How much slippage has occurred?

Answer: The impact of the reduction in FY 1985 from the proposed plan ($11.0 M) to $9.0 M is to delay a portion of the hardware procurements for the multiple-beam experiment (MBE). Such an experiment will be necessary to demonstrate the feasibility of the multiple-beam induction linac method. Operation of the full MBE in FY 1986 could be delayed by as much as three months and potential cost impact may be incurred due to the necessity to split certain procurements over two fiscal years.

18. What specific criteria must Phase I of the HIFAR program meet in order for consideration of the initiation of Phase II?

Answer: Adequate technical knowledge for initiation of Phase II of the HIFAR program is primarily dependent on successful demonstration of the multiple-beam experiments (MBE) in Phase I. In particular, initiation of Phase II would depend specifically on successful operation of the multiple-beam injector and first complement of modules of the MBE.

19. Assuming Phase I success, what is the estimated cost of Phase II of the HIFAR program?

Answer: The estimated cost of Phase II over a 3-year perod (FY 87-89) is between 60 and 80 million dollars. This includes both the base R&D, estimated at $4 M per year, and construction of the High Tempeature Experiment (HTE). A more accurate estimate of the cost of Phase II will be available following completion of the conceptual design of the HTE accelerator, which in turn depends on the full operational characteristics of the MBE.

20. What level of HIFAR program funding is estimated for each of FY 1984 and FY 1985 for LBL and LANL?

Answer: HIFAR program funding, including equipment funds, in FY 1984 for LBL is $3.7 M and for LANL is $1.0 M. Estimated funds for these laboratories in FY 1985 are $5 M for LBL and $2 M for LANL, with the remainder for other smaller contracts and undesignated purposes.

21. Please provide a copy of the revised HIFAR multi-year plan.

Answer: A copy of the HIFAR multi-year plan (LANL LA-UR-83-1717, May 1983) is attached.

Preprint LA-UR-83-1717

Title: HEAVY ION FUSION ACCELERATOR RESEARCH PROGRAM PLAN FOR FY84-FY-89

Author(s): Heavy Ion Fusion Staff, Los Alamos National Laboratory and
Lawrence Berkeley Laboratory (Compiled by R. O. Bangerter)

Submitted to: The Department of Energy's Office of Energy Research

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

HEAVY ION FUSION ACCELERATOR RESEARCH

PROGRAM PLAN FOR FY84-FY89

May 1983

*This work was performed under the auspices of the U.S. Department of Energy.

HEAVY ION FUSION ACCELERATOR RESEARCH

PROGRAM PLAN FOR FY84-FY89

MAY 1983

INTRODUCTION

In December 1981, Los Alamos National Laboratory, in its capacity as lead laboratory for heavy ion fusion (HIF), submitted to DOE a proposed "Plan for the Development of Heavy Ion Accelerators for Fusion Power, 1984-9" (Los Alamos report LA-UR-81-3730, hereafter referred to as the 1981 Plan). The objective of the 1981 Plan is to evaluate HIF as a commercial energy source. The evaluation requires the construction of an experimental accelerator capable of heating solid density material to a temperature of 50-100 eV. The accelerator and its associated experimental program are designated the High-Temperature Experiment (HTE).

The present document is a supplement to the 1981 Plan. Section I is a brief review of the motivation, issues, and status of the program. Section II gives the programmatic justification for the choice of accelerator technology. Section III outlines the issues that must be addressed to provide a basis for making decisions on the ultimate utility of accelerator technology for fusion applications. Section IV gives a detailed description of the R and D for FY84-FY89 with estimated schedules and costs.

SECTION I

MOTIVATION, ISSUES, AND STATUS

By 1976, theoretical work at the DOE Inertial Confinement Fusion (ICF) laboratories had shown that intense ion beams are well suited to the initiation of thermonuclear fusion. Specifically, the calculations showed that ion beam energies of several megajoules, delivered to a spot several millimeters in diameter over a period of ~15 ns would be adequate for ICF. These calculations assumed that the range of ions in high temperature (>100 eV) matter is roughly given by the theoretical expressions in textbooks[1] on this subject. However, this assumption has never been verified experimentally. The calculations also relied on a number of other assumptions about hydrodynamics and energy transport that have yet to be verified.

Current numerical simulations of targets indicate that the ion range should lie between 0.01 and 0.2g/cm^2 for acceptable performance. The upper limit of 0.2 g/cm^2 corresponds to a kinetic energy of about 10 MeV for protons and about 10 GeV for heavy ions such as lead. (See Appendix A for details.) Thus, deposition of a typical 3 MJ of ion energy in 15 ns requires a minimum beam current of 20 MA for protons, but only 20 kA for heavy ions. This illustrates the fundamental difference between light ion fusion and heavy ion fusion. Light ion fusion requires very large currents. Heavy ion fusion

uses high kinetic energy to achieve a thousandfold reduction in required current. Moreover, it is possible that additional target work will enable the use of even higher kinetic energies and lower currents.

High kinetic energy necessitates the use of multistage accelerator technology. Furthermore, multistage accelerator technology is also strongly preferred by the observation that such accelerators are reliable and efficient and have a long lifetime and a high pulse repetition rate. All of these characteristics are essential for commercial ICF.

In addition to these characteristics there are two fundamental requirements that must also be demonstrated before accelerators can be applied to fusion:

- Adequate beam quality characterized by high six-dimensional (6-D) phase-space density. In the absence of beam cooling mechanisms, Liouville's Theorem states that the phase-space density at the target cannot exceed the phase-space density at the ion source. The target constrains the three spatial dimensions of the occupied phase volume because of the requirements on focal spot size and pulse length. The finite apertures and chromatic aberrations of practical lens systems limit the momentum dimensions of the phase volume. One of the attractions of heavy ion accelerators is the fact that the available phase-space density determined by the target and lens constraints is orders of magnitude smaller than the phase-space density available from demonstrated ion sources. The real issue is how much the density is decreased by acceleration, beam manipulations, nonlinear space charge forces, accelerator imperfections, and/or instabilities.

- Containment and focusing of high charge-density beams. Given an adequately small phase-space volume, the volume must be properly shaped to remain in the accelerator and ultimately to meet the target requirements. The most stringent constraints on shaping arise from space charge forces and instabilities associated with high charge-density. Therefore, the constraints are most relaxed for high-energy, low-current beams -- further motivating the use of multi-stage accelerator technology.

There are three additional economic and engineering requirements that must be satisfied for commercial ICF:

- acceptable accelerator cost
- economical mass production of targets
- a practical reaction chamber

The principal accomplishment of the heavy ion fusion program to date has been an investigation of all of the above requirements. The accomplishments are documented in the reports of a large number of workshops and technical reviews (all favorable) listed in Table I.

TABLE I

REVIEWS OF THE HIF PROGRAM

• Workshops - Berkeley	1976, 1979
Brookhaven	1977
Argonne	1978
GSI, Darmstadt	1982
• Jason Study, JSR-77-41	1978
• Ad Hoc Experts Group on Fusion, 79-ETG-28 (SRD) (J. Foster)	1979
• EPRI Study, AP-1371 (K. A. Brueckner)	1980
• Oxford Symposium (J. D. Lawson)	1980
• Los Alamos Review (C. Longmire)	1981
• Jason Study, JSR-82-302	1982

For completeness we conclude this section with a brief summary of the current program elements.

- Evaluation and design studies for various HTE scenarios using accelerator systems based on one of the two leading technical approaches: r.f. linacs (using synchrotrons and/or storage ring accumulators) and the single-pass linear induction accelerator.
- Studies on the beam/target interaction. The status of this work was summarized by Bangerter.[2]
- Experiments to test the limits of high current beam transport systems.[3,4,5,6]
- Operation of heavy-ion sources of adequately high brightness.
- Construction and testing of induction linac modules applied to ion acceleration. The work at LBL[7] stresses the use of the long-pulse modules needed for the low-energy parts of an induction linac.
- Preliminary design studies for a high voltage injector for an induction linac.[8]
- Continued theoretical studies of key issues.

SECTION II

CHOICE OF TECHNOLOGY FOR R AND D PROGRAM

On page 4 of the 1981 Plan was stated: "The program plan that evolved between 1976 and 1979 called for the simultaneous development of the two most promising driver schemes--the rf/storage-ring technology and the linear induction accelerator (LIA) technology until a technical choice between the two could be made. A fast-track AIF program that could carry out a full program of theory and experiment in both of the leading approaches is generally not regarded as a credible possibility today. Therefore, the program described herein will include experimental and engineering work for one approach, the LIA. The work on the rf linac/storage ring approach will emphasize conceptual modelling and detailed simulation studies and relevant experiments at existing facilities."

The primary programmatic considerations which led to this choice of emphasis are given in the 1981 Plan. The proposed budget for FY84 was $7.5 M. The President's budget for FY84 is $5.0 M. At this level, it is necessary to focus strongly on a single approach in order to make significant progress. The requirement for experimental verification of theoretical and numerical simulations means that hardware must be developed in the next phase of the AIF program. In order to fund this development, under present budget constraints, one approach must be relegated to a very low level. Thus, the reasons for making a choice at this time are primarily programmatic. The choice itself, to concentrate on the LIA, has the same justification today as was given in the Plan:

"The Linear Induction Accelerator, combined with the high-current transport capabilities of multiple beams, has the characteristic of apparent simplicity that may result in a practical approach with cost savings. The key technical issues have been defined and can be answered at lower cost than those issues relevant to rf linac systems. These issues now require experimental (rather than additional analytical) exploration. Some of the hardware needed to make the first tests of beam current limits is in place. Thus, the LIA program is deemed appropriate for an early experimental test of the key accelerator concepts.

"The rf linac method requires further study and component development to determine if significant innovative solutions are available to reduce costs and guarantee the performance needed for the ICF applications. Key physics issues, such as stability limits and phase-space dilution factors (common to both rf and induction linacs, but in different form) have been defined. There are new requirements on the rings envisioned for the inertial fusion application, but the buy-in cost to test them is too high for now. Most of the basic know-how to build linac and ring systems has been well proven at accelerator installations around the world. Therefore, innovation in the technical use and cost reduction of this technology is considered appropriate at this stage. However, linac technology is also being studied abroad, notably in West Germany and in Japan, and there is a possibility that significant experiments on the current

limits in storage rings could be done on the Spallation Neutron Source at Rutherford, England, within a few years, or in less definitive way, at Argonne's booster ring, if operating time were available. A part of the effort will be used to participate in the international development of the rf/storage ring approach."

SECTION III

TECHNICAL ISSUES AND RESEARCH REQUIREMENTS

III-A. GENERAL DISCUSSION

From the discussion in Section I we note that the promise of accelerator fusion rests on a number of assumptions that can be summarized as follows:

1. It is possible to build an efficient accelerator, at reasonable cost, that can generate high-energy (>1 MJ) ion beams occupying a small 6-dimensional phase-space volume.

2. The beams from such an accelerator can be focused over a distance of several meters onto a small target located in a reaction chamber. (Small 6-dimensional phase-space volume is a necessary, but not sufficient condition, for this to occur.)

3. Our present calculations adequately describe ion energy deposition.

4. The hydrodynamic and thermonuclear behavior of the target is reasonably well described by our numerical simulations.

5. Targets corresponding to our numerical models can be mass produced at acceptable cost.

6. A reaction chamber can be built that economically converts the target products into useful energy and produces target fuels not adequately occurring in nature.

All six assumptions must be tested to provide a basis for sound decisions. The OER accelerator program leading to completion of the High Temperature Experiment (HTE) will test the first three assumptions. In a memo dated June 21, 1982, Herman E. Roser, Assistant Secretary for Defense Programs, and Alvin W. Trivelpiece, Director of the Office of Energy Research, agreed to retain target design activity in Defense Programs. Since Defense Programs also supports target fabrication and reactor studies, the last three assumptions are also being evaluated.

III-B. TECHNICAL REQUIREMENTS FOR THE HTE

In order to ensure that the HTE supply an adequate data-base for proceeding with confidence to a larger-scale application of accelerator technology to ICF, we identify six key properties of the HTE that must approach in scale the corresponding properties for a fusion driver. Exactly how close an approach is needed is a matter of judgment and depends on a trade-off between cost and confidence. To be definite in what follows, we adopt a factor of three as a reasonable quantitative scale factor between the needs for a driver and the required performance of the HTE. In order, the six desired conditions are:

- To Test Accelerator Physics and Engineering:

(1) Number of Independent Components: As explained in the introduction, there are two principal issues -- demonstration of adequate 6-D phase space density and containment of high charge-density beams. Since ample 6-D phase space density is available at the ion source, demonstration of high phase space density is equivalent to demonstration that emittance growth in both the transverse and longitudinal phase volumes is not excessive. (For a quantitative discussion of allowable emittance growth see Ref. 9.) Emittance growth can be caused by a number of mechanisms such as injection mismatches, instabilities, and random field errors in both the transverse and longitudinal directions. Growth due to mismatches is expected to be rapid and, if serious, should be observable in the early stages of acceleration. By a proper choice of parameters it may also be possible to stimulate and observe certain deleterious instabilities in a relatively short accelerator.

By contrast, the growth due to random errors should be proportional to the square root of the number of focusing elements and accelerator pulsers; it cannot be observed in a short accelerator. As an example, we consider an induction linac test accelerator with N_e electric quadrupoles, N_m magnetic quadrupoles, and N_p accelerator pulsers. Because of the square-root relation, therefore, it is desirable to have:

$$(N_e)_{test} \gtrsim 0.1\ (N_e)_{ICF\ driver}$$
$$(N_m)_{test} \gtrsim 0.1\ (N_m)_{ICF\ driver}$$
$$(N_p)_{test} \gtrsim 0.1\ (N_p)_{ICF\ driver}$$

(2) Betatron Wavelength: For partly related reasons, it is desirable to have the number of betatron wavelengths, N_β, along either the test or driver accelerator not grossly different; hence:

$$(N_\beta)_{test} \gtrsim 0.3\ (N_\beta)_{ICF\ driver}$$

(3) Space Charge Limit: Since both the HTE and a driver would operate close to the space charge limit, the containment of high space charge density beams is tested at full scale.

- To Test Beam Focusing:

(4) Lee Parameter: For focusing experiments the important quantities are beam stiffness and space charge forces. A single parameter that measures beam stiffness relative to space charge forces was devised by Edward P. Lee of LBL. This parameter is given by $L = (I_p/I_A)(m_e/m_i)(Z^2/\beta^3)$ where I_p, I_A, m_e, m_i, Z, and β are beam particle current, Alfven current coefficient = 17000 amps, electron mass, ion mass, ion charge state, and (ion speed)/(speed of light). In order to perform meaningful beam focusing experiments, L for the HTE should not be much smaller than L for a fusion driver. We adopt the following specific criterion

$$L_{test} \gtrsim 0.3\ L_{ICF\ driver}$$

- To Test the Beam-Target Interaction:

(5) Beam Plasma Frequency: For validation of the beam-target interaction, both beam and target parameters should be appropriately chosen. For the beam, the beam plasma frequency, ω_{pb}, is an important quantity. It appears in growth rates for beam-plasma instabilities. Thus it is desirable to have

$$(\omega_{pb})_{test} \gtrsim 0.3\ (\omega_{pb})_{ICF\ driver} .$$

(6) Temperature: All important quantities of interest describing the target material are functions of temperature, density, and composition. The density and composition can be easily varied over a wide range. Therefore the matter temperature, T, becomes the critical quantity. ICF will probably require 150 < T < 300 eV in the beam deposition region. Thus it is desirable that

$$T_{test} \gtrsim 50\ eV .$$

The criteria listed above are not completely independent. In fact for typical induction linac scenarios the last criterion, $T \gtrsim 50$ eV, is sufficiently stringent that all of the other criteria are automatically satisfied. In principle, therefore, all of the criteria can be combined into a single milestone:

- Production of a temperature of 50-100 eV in a dense ($n_e \gtrsim 10^{22}/cm^3$) target material by ion beams from a multi-modular accelerator;

which, by itself, defines the high-temperature experiment (HTE). This temperature cannot be achieved unless the accelerator, bunching, focusing, and the beam-target interaction are successful.

III-C. CONCLUSIONS

The range of accelerator parameters being explored for the HTE (See Section IV-A) satisfies all of the above conditions and should lead to a meaningful test of acceleration, focusing and the beam-target interaction. It is an important and relatively recent conclusion, after some years of study, that an HTE, based on these parameters, although much smaller than a driver, can come so remarkably close in scale to matching these six features. In part, this arises from the fact that an ion induction linac by its nature requires a high density of independent accelerating modules and focussing lenses at the low velocity end compared with a relatively low density as the kinetic energy is increased to higher and higher values. The choice of an ion mass well below A = 200 and a velocity one-third of that appropriate to a driver, are also important for reducing size and cost while retaining the desired physics and engineering features.

The 1982 JASON review referred to in Table I concurs with this assessment. The report states:

"The proposed facility for the HTE has beam current, total energy, and power parameters which will allow an important check on the theory of space charge limited propagation in drivers; will develop the technology of drivers and allow a more reliable estimate of the cost of a full-scale driver to be made; will allow experiments to be performed on beam propagation in a reactor environment; and will check for any effects in coupling physics that have been so far overlooked...

"The proposed National Plan for HIF seems to be a sensible and minimal next step in HIF. With the addition of an experimental program on the interaction of high energy heavy ions with cold matter, and an appropriate theory effort, it should go a long way toward determining the potential of HIF for energy production."

SECTION IV

ACCELERATOR R AND D PLAN FOR FY 1984, 1985, AND 1986

IV-A. GOALS AND BACKGROUND

The major goal of the 6-year program is to establish a physics and engineering data-base sufficient to allow firm evaluation of the prospects of the heavy-ion accelerator technology for production of civilian fusion power. Three years of intensive R and D (Stage I) are needed in FY 1984-6 to establish a design and cost basis -- backed by engineering prototypes and a validation of the accelerator-physics feasibility -- for construction of a significant High Temperature Experiment (HTE) in the following 3 years (Stage II).

The HTE presents many of the problems of a full-scale driver, except for overall size and cost. The particle energy, beam energy, and ion mass are all reduced in the interests of economy but essentially all the desired physics and engineering aspects remain pertinent. All of the requirements given in Section III are satisfied. The beamlets pass through the same processes of launching into an induction linac, bunch length control during acceleration, final bunch compression, and final focusing in both systems, in addition to being transversely focused near the space charge limit throughout. It should be noted that after the HTE system is built, some operating flexibility will exist, because the focusing system can work over a range of particle energies and currents; also the beam energy-gain and current amplification schedules may be varied by reprogramming the firing times of induction module pulsers.

It is appropriate here to give a brief description of example parameters for the HTE based upon current conceptual studies. It should be stressed that these studies are still in progress so that this example should be treated as one that represents the current state of thinking. Example parameters are as follows:

Ion:	Sodium
Beam Energy:	3 kJ
Kinetic Energy:	100 MeV
Focal radius:	1 mm
Pulse Length at Target:	10 ns

As now envisaged, the HTE will start with a 6-Amp, 5-μs current pulse, and end with a 300-Amp, 100-ns pulse at the output of the accelerator, followed by a drift section where the beam bunches to a 3-kA, 10-ns pulse at the target. The focusing system will occupy one half of the length of the approximately 400-meter long machine, with electrostatic lenses used in the first third and permanent magnet lenses in the rest of the machine and the bunching lines. The lens aperture diameter will be a constant 3-cm per beamlet, and the half-period of the focusing structure will increase along the machine. The focusing structure is nested inside the induction modules, alternating with the insulators through which the accelerating field is applied.

IV-B. RESEARCH AND DEVELOPMENT, STAGE I (FY84-FY86)

Three major R and D program elements are required:

1. Engineering R and D for the High Temperature Experiment (HTE): pre- and full-prototype subsystems for the HTE. This will continue through the full three year period. The HTE final design decisions, needed late in FY86, will rely heavily on the results and cost information developed by this R and D.

2. Physics experimentation on a Multiple Beam Accelerating System Multiple Beam Experiment (MBE). The design of this system must be committed in FY84 so that the experimental results can be available for evaluation late in FY86. Thirty accelerating units (each with 10 modules) and thirty focusing arrays are needed for a satisfactory beam test.

3. Design of the HTE: Exploration of various accelerator strategies to achieve suitable beam-energy-gain and current-amplification schedules will continue for the 3-year period. This activity both guides, and is guided by, strong interaction with the first two elements.

All three elements will be backed by an aggressive theoretical and simulation program to further understand fundamental properties of transverse and longitudinal dynamics in the proposed systems and to guide the design and experimental work.

The breakdown of the costs and schedules are given in Section IV-C.

IV-B.1. Engineering R and D for the HTE

The R and D Plan leading to the HTE is based on developing components and subsystems which can be used directly or easily scaled to the HTE, and in minimizing their costs. The actual design of the HTE will proceed in parallel with the hardware development and will, as it evolves, quite strongly affect the hardware decisions. During the Stage I three-year period, the two major tasks are:

Task 1: (FY84-86) Accelerating Structures

Determine the attainable accelerating fields in the induction units: risetime, jitter, breakdown strength, graininess in approximating shaped waveforms, and reliability. Minimize costs.

Task 2: (FY84-86) Multiple-Beam Focusing Arrays

Determine the attainable focusing fields in multiple beam electric and magnetic quadrupole arrays, including mechanical tolerances and field nonlinearities, to specify focusing geometry and induction unit aperture.

A number of full-scale induction modules representative of those required at several locations along the HTE accelerator will be fabricated and tested to evaluate their performance. The attainable risetimes, jitters, and shaped waveforms synthesized by varying the firing times of many identical modules will be measured and evaluated in order to determine the maximum amount of graininess and other disturbances which would be tolerable to the beam. The core drive currents and risetimes will determine the choice of pulse-forming circuitry and switches: for long pulses (>1μs) a lumped element line switched by ignitrons is satisfactory; for submicrosecond pulses thyratrons are needed to provide a short risetime and low jitter. A distributed element pulse-forming line may become preferable for pulses near 100 ns. After the initial bunch launching into the induction linac, the required waveforms tend toward constant voltage pulses, in which case it is permissible to drive as many cores as possible with one pulser, whereas in the front part of the machine waveform requirements will determine the required number of pulsers.

At this time, metallic glass magnetic cores appear preferable. A development program in conjunction with the manufacturer needs to be reactivated to improve the material packing fraction and the interlaminar insulations. Ideally, the manufacturer would supply finished cores directly, without need for a separate insulating process.

The developmental program on the focusing arrays will proceed in parallel with acceleration module development. The goal is to arrive at precise and stable structures which are nested within the heavy induction modules but are mechanically independent of them in such a way that they can be aligned (and realigned) to a tolerance of a few mils. A cryogenic pumping system will be an integral part of the array, with the ability to reach 10^{-7} Torr in the highest pressure location.

At this time, the anticipated costs of the HTE accelerator components are uncertain; a major goal of the R and D program is to minimize and to better define these costs. The focusing structure, the mechanical support for the cores, and the vacuum insulator will cost about $50 k/m, the rare-earth cobalt permanent magnets, where used, will cost about $25 k/m, the induction cores about $25 k/m, and the pulsers about $25 k/m. A number of cost reduction efforts have been started, such as the development of large castable polymer concrete insulators with integral feed throughs; investigation of improved or cheaper methods for final beam focusing will continue as parts of the base program.

IV-B.2. R and D on the Multiple-Beam Experiment

Acceleration of an array of multiple intense ion beams is an essential prerequisite to proceeding with HTE construction, to ensure that both physics and hardware expectations are met in the actual beam environment. Progress to this end requires the following tasks:

Task 3: Beam Transport Physics

Determine the beam transport limits experimentally, using precise fields and ample diagnostics. Measure the beam size as a function of current and emittance for various machine settings to find optimum transport parameters.

Task 4: Injector

Develop a high-brightness, high-voltage Na^+ injector and matching section for multiple beams. Needed early FY85.

Task 5: System Integration and Performance Verification - the MBE

Assemble the injector, accelerating units, focusing structures, and diagnostics into a system and verify that it performs as expected and that the bunches can be transversely and longitudinally controlled without significant dilution, using available and economic hardware. To allow significant test results to be ready by the end of FY86 based on experience with 30 accelerating units and 30 focusing arrays, the choice of major component designs will be selected in the latter part of FY84 based on the then best information available from Tasks 1 and 2.

Task 6: Diagnostics

Develop accurate diagnostics and correction systems and determine how many are required. MBE provides crucial test facility.

The MBE transport and accelerating system will consist of 30 accelerating units, each containing 10 independent modules, for representative locations of the HTE as it is now conceived. Each accelerating unit and its integral focusing array will be chosen to fit one of 5 evenly spaced half periods of the focusing lattice, starting at 30-cm length and increasing by 10-cm increments to 70 cm. Approximately 0.5 volt-seconds of induction core will be used per meter of length, resulting in a unit outside-diameter slightly greater than 1 meter and similar to the long-pulse induction unit constructed at LBL in FY83. The total machine length will be 30 meters, including 15 meters of alumina accelerating column and 15 meters of focusing arrays. These will be surrounded by 30 meters of induction cores. Most of this hardware could probably be repackaged for use in the HTE.

An important goal of the MBE will be to determine if a sufficiently precise focusing system can be built which would permit omission of most of the diagnostics and beam correction elements in the HTE. The required magnetization tolerance is believed to be about 1 percent and does not pose severe difficulties. A major difference between the focusing in the multiple beam array and that in the ongoing single-beam transport experiment (SBTE) is that the physical clearance between the beam and the focusing structure has to be minimum in the array instead of ample as in the transport experiment. Some knowledge of the halo of particles around the dense central part of the beam, and whether the halo re-forms if it is scraped off, will be gained from the SBTE and will be a guide for the HTE lattice. A question which can best be answered experimentally is whether beam loss in a large array will lead to electrical breakdown in an electrostatic quadrupole system.

The dominant effects are those of a single focusing channel on its own beamlet, and these will be investigated near the exit of the SBTE where the beam is well characterized and instrumented. The interaction of beamlets with each other, however, which depends partly on the physical design of the lattice, and, for electric quadrupoles, on the electrical circuit connecting the array to an external voltage source, must be studied experimentally. Some of the beam tests for a multiple beam array could be done with a small number of beamlets, representing some edge beamlets and some interior beamlets.

Concurrently, development will proceed on a high voltage gun for injecting a high current Na^+ beam into an induction linac. At any location within an induction linac, the beam varies in current and energy as functions of time in a prescribed manner intended to ensure stable transport of all particles within the bunch, as well as a controlled amount of velocity tilt for bunch length control. In principle, an ion gun could match into the induction linac at any point if the current, voltage, and beam emittance are at the prescribed values. Because of limits and constraints imposed by the transport requirements, the initial stages of inductive acceleration tend to be disproportionately expensive. A preliminary estimate comparing the costs of an induction accelerator starting at 2 MeV with one starting at 10 MeV indicated a significant savings for the higher injector energy case. In either the 2 MeV or the 10 MeV injector case, a further significant savings may result from tailoring the injected current and voltage profiles while maintaining matching into the focusing system; this option is being pursued theoretically. The cost per volt of induction acceleration is a decreasing function of energy, (decreasing rapidly to approximately 50 cents per volt at 50 MeV in the HTE induction linac): conversely, the cost of an injector is an increasing function of voltage. Consequently the greatest relative savings are possible at the low energy end, and worthwhile savings would result from intermediate voltage choices if the 10 MeV goal is too difficult to reach.

IV-B.3. The Design of the HTE

This is a continuation of an effort that has been in progress for the past year and which is defined as follows:

Task 7: Design of the HTE: Still in the physical conceptual stage with choices guided by preliminary engineering concepts and costs. The effort will extend through FY86 and, incorporating input from the results of preceding tasks, will become focussed to a preliminary engineering design at the end of FY86.

In contrast with many other accelerator systems, an ion induction linac for HTE has a very large safety margin in regard to acceleration of the beam currents in question. The major physics constraint enters through the limits encountered in the transport system. Instead, therefore, of seeking for a balance between competing physical constraints, the procedure for optimizing the design must rely heavily on cost trade-offs between one set of stressed and another set of under-stressed components of the system (Ref. 1979). Hence derives the crucial importance of combined input from the progress of the hardware Tasks 1-6.

The central goal of the design study is establishing an optimum energy-gain schedule and current-amplification schedule along the accelerator with a reasonable match to, and hence definition of

a) The injector kinetic energy, and injector energy or current ramp, and

b) The most desirable current and energy ramp needed for correct bunching in the final transport to the target.

While the tentative choice of ion-mass and charge-state (Na^{+1}) seems close to optimal, the array of other parameters to be picked still presents a large dimensionality. Completion of Task 3 in FY84 will serve to restrict further the choices. Tasks 1 and 2 will provide the input to establish an optimum engineering design, while the physics credibility of that design must rest on completion of the remaining Tasks 4-6 (i.e., MBE).

IV-C. COSTS AND SCHEDULES (All in FY84 K$)

This section shows a breakdown of the costs, activities and schedules for the Stage-I R and D program. Because the MBE represents a significant hardware investment in this period, an approximate breakdown of its costs is displayed separately (C-1). Activities related to the construction of HTE which fall within the Stage I time-frame are also displayed. Finally, a tentative HTE construction schedule is given (C-7).

IV-C.1. Major Cost Components of the Multiple Beam Experiment (MBE) Program

Metglas cores with interlaminar insulation $12 K/ton x 200 tons		2,400 ($K)
Alumina insulator columns 40K/m x 15 meters		600
Electrostatic focusing array 50K/m x 12 meters		600
Permanent magnet focusing array 100K/m x 18 meters		1,800
Pulsers 5K/pulser x 10 pulsers/m x 30 meters		1,500
Cryopumping system		500
Packaging of assembly		1,600
Ion Source and Injector		2,000
	Total	11,000 ($K)
Design and Engineering at 40 percent		4,400
		15,400 ($K)
Contingency at 36 percent		5,500
	Total	20,900 ($K)

HEAVY ION FUSION ACCELERATOR RESEARCH

IV-C.2. Stage-I R and D Activities and Costs

FY 84		5000 (K$)
Base Program	3000 (K$)	
Theoretical Studies		
Conceptual Design Studies		
Core and Insulator Development		
Beam Diagnostic Development		
Beam Transport Physics		
Multiple Beam Experiment R and D	2000 (K$)	
Injector Design and Construction		
Core and Insulator Procurements		
Induction Unit Development		
Focusing Array Design and Development		
Pulser Design and Development		
Freeze Specs. of MBE Components		
FY85		11000 (K$)
Base Program	4000 (K$)	
Theoretical Studies		
Conceptual Design Studies		
Beam Diagnostics Development		
Core and Insulator Development		
Beam Transport Physics		
Multiple Beam Experiment R and D	7000 (K$)	
MBE Injector Completion and Operation		
MBE Induction Unit and Focusing Array Tests		
Acceleration Structure Tests and Development		
Complete Construction of Induction Units and Focusing Arrays for MBE		
FY86		17000 (K$)
Base Program	5000 (K$)	
Theoretical Studies		
Conceptual Design Studies		
Beam Diagnostics Development		
Core and Insulator Development		
Beam Transport Physics		
Multiple Beam Experiment R and D	12000 (k$)	
Complete Installation of Induction Units and Focusing Arrays		
Determine Performance Characteristics of Components and System		
Provide R and D Results to freeze HTE Component Design		
Conduct Multiple Beam Transport Studies and Beam Diagnostic Measurements		

HEAVY ION FUSION ACCELERATOR RESEARCH IV - C.3. TABLE OF COSTS - M$				
	FY 84	FY 85	FY 86	FY 87 - 89
BASE PROGRAM	3.0	4.0	5.0	
RANGE - ENERGY	0.15			
INDUCTION ACCEL. & BEAM TRANSPORT	0.85	4.0	11.0	
MULTIPLE BEAM INJECTOR	1.0	3.0	1.0	
TOTAL R & D	5.0	11.0	17.0	
HIGH TEMPERATURE EXPERIMENT (HTE)			0.8*	60 - 80

*PE & D FUNDS

HEAVY ION FUSION ACCELERATOR RESEARCH

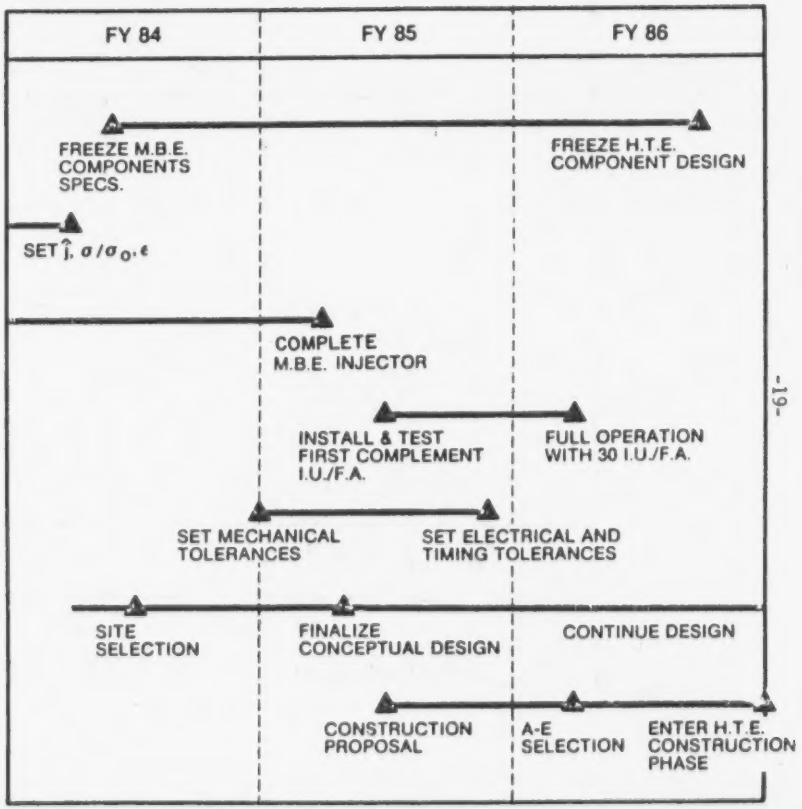
STAGE I
R & D SCHEDULE

PROGRAM MILESTONES

Engineering R & D
- Induction Units and Focusing Arrays
- Single Beam Transport Experiment

Multiple Beam Experiment
- Injector
- Induction Units and Focusing Arrays (I.U./F.A.)

High Temperature Experiment Conceptual Design
- Physics Design
- Engineering Design
- Pre-construction



HEAVY ION FUSION ACCELERATOR RESEARCH

IV-C.5. Stage-I R and D FY84-86 Chronology

Decision Dates ● / Milestones ▲		
●	Single Beam Transport Experiment sets $\hat{J}$, σ/σ_0, ϵ *	Nov. 1983
●	Freeze Multiple Beam Experiment component specs.	Mar. 1984
●	Set mechanical tolerances on HTE components	Oct. 1984
▲	Complete Multiple Beam Experiment injector	Jan. 1985
▲	Install first group of induction units and focusing arrays	Mar. 1985
●	Set HTE electrical and timing tolerances	Sept. 1985
▲	Complete installation of induction units and focusing arrays	Jan. 1986
●	Freeze High Temperature Experiment component design	Aug. 1986
●	Complete High Temperature Experiment accelerator preliminary design	Oct. 1986

* $\hat{J}$ = peak current density
σ/σ_0 = phase advance per cell with space charge/single particle phase advance per cell
ϵ = transverse beam emittance

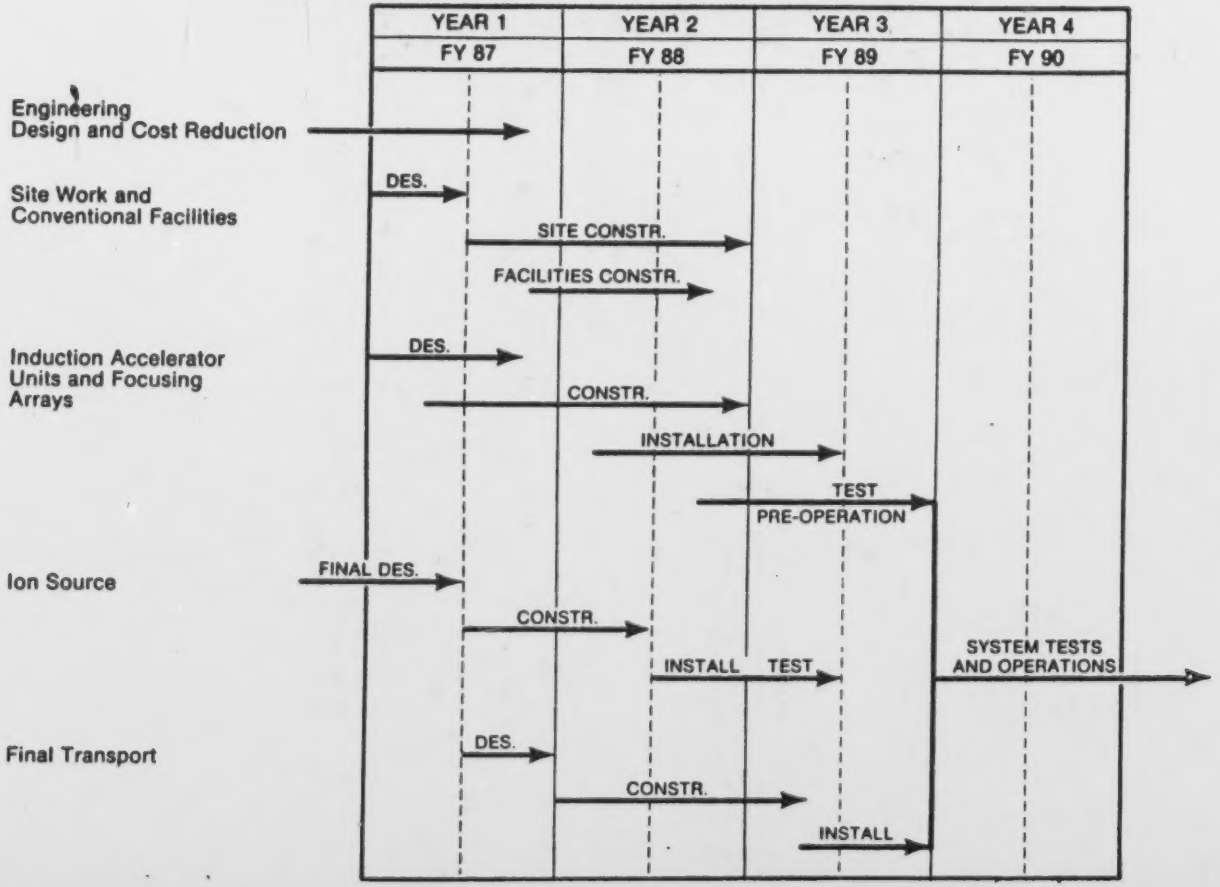
HEAVY ION FUSION ACCELERATOR RESEARCH

IV-C.6. High Temperature Experiment Accelerator Pre-Construction Decision Dates (FY83-FY86)

Site selection	March 1984
Construction proposal	March 1985
A and E selection	Jan. 1986
P E and D funds	June 1986
Order cores and insulators	July 1986
Acceleration/Transport preliminary design and cost reduction	Ongoing throughout 1986

HEAVY ION FUSION ACCELERATOR RESEARCH

HIGH TEMPERATURE EXPERIMENT (H.T.E.)
ACCELERATOR CONSTRUCTION SCHEDULE (Preliminary)



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APPENDIX A

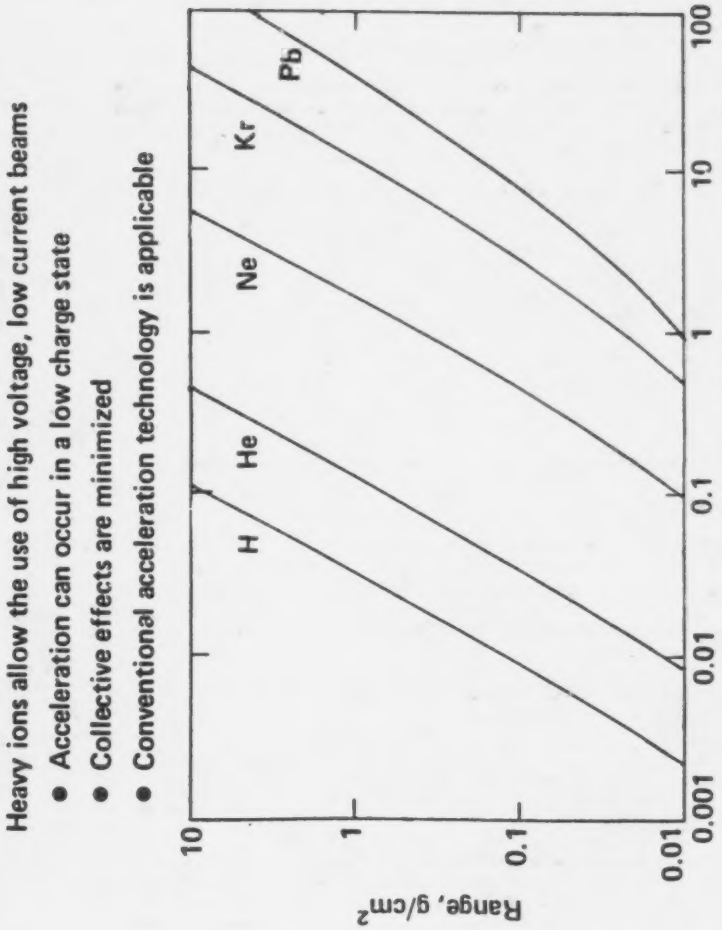

Fig. 1 Ion range in g/cm^2 as function of ion kinetic energy. These curves are based on aluminum target material at a temperature of 200 eV and density of 0.2 g/cm^2, corresponding to typical target conditions.

2.0 Isotope Preparations

22. What is the Research Materials Collection (RMC)?

Answer: The RMC is an inventory of samples of separated stable isotopes that are allocated to investigators on a loan basis for fission and fusion energy technology research. This collection has been built up over the years at a production cost of approximately $18M, more than half of which is out on loan to researchers at any given time. A continuing upgrade/maintenance effort is required both as to sample quality and replacement of processing losses. The RMC is valued as a national resource.

23. What are the actual and estimated revenues from the sale of isotopes for the period FY 1981 - FY 1985? How much was received from the sale of isotopes to (a) DOE laboratories, (b) universities, (c) industry, (d) other DOE programs, and (e) other agencies?

Answer: Actual and estimated total revenue from the sales of stable isotopes by year is:

	Budget Authority (M$)				
	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Total Stable Isotopes Sales Revenue	3.96	3.74	3.05	3.22	3.45
DOE Laboratories	0.11	0.17	0.11	0.17	0.18
Other Federal Programs	0.05	0.03	0.08	0.07	0.07
Other Domestic	2.65	2.33	1.80	1.91	2.05
Foreign	1.15	1.21	1.06	1.07	1.15

Sales data by the requested breakdown are not normally maintained.

24. What is the pricing policy?

Answer: The pricing policy governing the sale of stable isotopes is determined to effect full cost recovery. This cost is defined as the cost the government incurred to produce the sample in the year it was produced.

25. What is the current inventory? How is it decided which isotopes to produce and when to produce them?

Answer: Current inventories of stable isotopes are:

	Budget Authority $	Amount (grams)
Sales Inventory	6,291,681	2,973
Research Materials Collection	18,534,374	28,381

Isotope production schedules are determined by the historical demand patterns plus discussions between the Oak Ridge staff and the various customer groups. In addition, schedules can be adjusted to meet special needs. In order to facilitate the conduct of research, an effort is made to maintain as complete an inventory as possible.

26. What is the role of Mound Laboratory in the program? Why are funds being requested for decontamination and decommissioning?

Answer: Before 1979, Mound Laboratory was used to separate small quantities of certain rare actinide isotopes which were sent to ORNL for sale through the Isotope Sales Office. The demand for these isotopes was very low, and because available inventories were considered adequate it was decided in 1979 to cease production. Because the Nuclear Sciences subprogram was the last one to use that lab space it must either fund an annual laboratory maintenance and radiological surveillance effort or pursue the cleanup of the laboratories so the space can be used for other purposes and terminate the Nuclear Sciences obligation.

G. Applied Mathematical Sciences Subprogram

1. **What is the detailed budget structure of the Applied Mathematical Sciences subprogram? What types of work are funded by each of these budget categories?**

   Answer: The Applied Mathematical Sciences subprogram is divided into two major categories: Supercomputing Research and Energy Sciences Advanced Computation. Supercomputing Research is divided into three areas: Analytical and Numerical Methods, Information Analysis Techniques, and Advanced Computing Concepts. The areas of research funded under each of these topics is detailed on pages 2-7 of DOE/ER-0157/1, "Summaries of the FY 1983 Applied Mathematical Sciences Research Program," a copy of which is attached.

   The Energy Sciences Advanced Computation activity is intended to provide access to advanced supercomputing systems for contractors in the Office of Energy Research's High Energy and Nuclear Physics, Basic Energy Sciences, and Biological and Environmental Research programs.

2. **For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.**

   Answer: The operating breakdown for the categories identified in Question 1 are as follows:

APPLIED MATHEMATICAL SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0402 APPLIED MATHEMATICAL SCIENCES					
KC0402010 ANALYTICAL AND NUMERICAL METHODS	4,373	6,800	6,777	7,000	8,500
KC0402020 INFORMATION ANALYSIS TECHNIQUES	1,573	1,600	1,608	1,770	3,620
KC0402030 ADVANCED COMPUTER SYSTEMS CONCEPTS	5,000	5,000	4,900	5,100	8,330
KC0402040 SPECIAL PROJECTS	275	411	565	800	800
KC0402050 ADVANCED COMPUTATION	0	0	0	0	7,000
TOTAL	11,221	13,811	13,850	14,670	28,250

The capital equipment funds are not broken down below Applied Mathematics. These totals are as follows:

CAPITAL EQUIPMENT	706	800	800	970	1,500

3. **How much of the FY 1985 Advanced Mathematical Sciences budget request is for support of programs formerly funded by the DOE Magnetic Fusion Energy Program, or by any other DOE program?**

Answer: None of the Advanced Mathematical Sciences budget is for support of programs formerly funded by other DOE programs.

4. **Please provide a listing of each of the current and planned Research Computing Facilities (RCF's). For each of the RCF's, please provide the date of establishment, equipment inventory, and a description of the research supported, as well as a copy of the latest annual report.**

Answer: The "canonical" RCF consists of a DEC Vax 11/780 system with 4 megabytes of memory, 600 megabytes of disk, a floating point accelerator, a tape drive, a BBN C/30 Interface Message Processor for accessing the Defense Data Network (originally, the ARPANET), various terminals, printers, plotters, etc. The following list gives an indication of the current configurations by laboratory.

SITE	EQUIPMENT	YEAR ESTABLISHED
Ames Lab	Vax 11/750 and graphics workstation	FY 1984
Argonne	Vax 11/780 and workstations	FY 1981
Brookhaven	PDP 11/44	FY 1981
Los Alamos	Vax 11/750	FY 1983
LBL	Vax 11/780 and workstations	FY 1979
LLNL	Vax 11/780	FY 1983
NYU/Courant	Vax 11/780(2) and FPS 164	FY 1979
ORNL	Vax 11/780	FY 1983
PNL	Vax 11/780 and graphics workstation	FY 1980
SANDIA	(No RCF supported by AMS program)	

Although not all the laboratories have all the components, most have enough equipment to be able to exchange software and messages amongst themselves and with the many universities and other government laboratories on the network. No new RCF sites are being planned for at this time.

The description of the research activities supported on these RCF's is detailed on pages 6 and 7 of DOE/ER-0157/1, "Summaries of the FY 1983 Applied Mathematical Sciences Research Program", a copy of which is attached.

Because these facilities are small, minicomputer-based operations, they are not required to issue annual reports.

5. **For the period FY 1981 - FY 1985, please identify, by budget category and by Research Computing Facility, that portion of Applied Mathematical Sciences funding that goes for the support of the RCF's at DOE national laboratories and universities.**

Answer: The funding associated with Research Computing Facilities by laboratory and university is as follows:

RESEARCH COMPUTING FACILITIES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
OPERATING EXPENSES					
KC0402040 SPECIAL PROJECTS					
ARGONNE NATIONAL LAB	$ 75	$ 100	$ 100	$ 100	$ 100
LAWRENCE BERKELEY LAB	150	100	100	100	100
LAWRENCE LIVERMORE NAT LAB	0	25	100	100	100
LOS ALAMOS NATIONAL LAB	50	50	100	100	100
NEW YORK UNIVERSITY	50	100	100	150	150
OAK RIDGE NATIONAL LAB	0	35	65	100	100
PACIFIC NORTHWEST LABS	0	100	100	100	100
CAPITAL EQUIPMENT					
AMES LABORATORY	48	0	25	75	50
ARGONNE NATIONAL LAB	75	50	100	280	100
BROOKHAVEN NATIONAL LAB	0	0	0	50	0
LOS ALAMOS NATIONAL LAB	80	40	30	50	100
LAWRENCE BERKELEY LAB	150	60	185	30	100
LAWRENCE LIVERMORE NAT LAB	3	200	135	85	900
NEW YORK UNIVERSITY	250	250	250	300	300
OAK RIDGE NATIONAL LAB	30	200	75	50	50
PACIFIC NORTHWEST LABS	70	0	0	50	0

6. **For the period FY 1981 - FY 1985, please provide, by budget category and company, the amount of Applied Mathematical Sciences funding going to industry.**

Answer: Please see the table below for requested information.

APPLIED MATHEMATICAL SCIENCES
INDUSTRY
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0402 APPLIED MATHEMATICAL SCIENCES					
KC0402010 ANALYTICAL & NUMERICAL METHODS					
OPERATING EXPENSES					
SCIENCE APPLICATIONS	$ 65	$ 65	$ 65	$ 85	$ 75
KC0402040 SPECIAL PROJECTS					
OPERATING EXPENSES					
RECON	0	2	0	0	0

7. For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Applied Mathematical Sciences funding going to DOE laboratories.

Answer: Please see the table below for requested information.

APPLIED MATHEMATICAL SCIENCES
LABORATORIES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0402 APPLIED MATHEMATICAL SCIENCES					
KC0402010 ANALYTICAL AND NUMERICAL METHODS					
OPERATING EXPENSES					
AMES LAB	$ 225	$ 250	$ 300	$ 400	$ 475
ARGONNE NATIONAL LAB	750	800	850	900	950
BROOKHAVEN NATIONAL LAB	175	300	325	340	355
LAWRENCE BERKELEY LAB	325	500	580	580	650
LAWRENCE LIVERMORE NAT LAB	175	175	175	175	200
LOS ALAMOS NATIONAL LAB	288	300	300	315	350
OAK RIDGE NATIONAL LAB	350	350	360	380	470
SANDIA CORP	165	180	200	210	225
SANDIA LAB, LIVERMORE	325	350	400	435	475
KC0402020 INFORMATION ANALYSIS TECHNIQUES					
OPERATING EXPENSES					
BROOKHAVEN NATIONAL LAB	225	125	275	290	320
LAWRENCE BERKELEY LAB	533	450	600	450	525
OAK RIDGE NATIONAL LAB	315	315	325	340	350
PACIFIC NORTHWEST LABS	500	400	408	400	400
KC0402030 ADVANCED COMPUTER SYSTEMS CONCEPTS					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	850	875	1050	1150	1550
LAWRENCE BERKELEY LAB	325	300	250	200	200
LAWRENCE LIVERMORE NAT LAB	425	450	475	500	650
LOS ALAMOS NATIONAL LAB	375	450	545	700	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0402040 SPECIAL PROJECTS					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	75	100	100	100	100
LAWRENCE BERKELEY LAB	150	100	100	100	100
LAWRENCE LIVERMORE NAT LAB	0	25	100	100	100
LOS ALAMOS NATIONAL LAB	50	50	100	100	100
OAK RIDGE NATIONAL LAB	0	35	65	100	100
PACIFIC NORTHWEST LABS	0	100	100	100	100

8. **For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of Applied Mathematical Sciences funding going to universities.**

Answer: Please see the table below for requested information.

APPLIED MATHEMATICAL SCIENCES
UNIVERSITIES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0402 APPIED MATHEMATICAL SCIENCES					
KC0402010 ANALYTICAL AND NUMERICAL METHODS					
OPERATING EXPENSES					
ATLANTA UNIVERSITY	$ 0	$ 0	$ 62	$ 67	$ 70
CALIF UNIV OF BERKELEY	250	332	363	97	100
CALIFORNIA INST OF TECH	163	163	249	259	271
CLAREMONT COLLEGES	- 2	0	0	0	0
CLARKSON COLLEGE OF TECH	0	0	19	0	25
COLUMBIA UNIV	0	0	0	57	0
CORNELL UNIV	0	0	166	225	236
DELAWARE UNIV OF	35	46	0	0	0
DENVER UNIV OF	0	- 1	0	0	0
ILLINOIS UNIV OF	220	220	220	184	194
INDIANA UNIV	0	59	85	92	90
KENT STATE UNIV	185	175	199	103	108
MARYLAND UNIV OF	0	75	114	138	146
NEW YORK UNIV	1350	800	1100	1150	1250
NORTHWESTERN UNIV	73	83	95	100	0
PRINCETON UNIV	0	- 5	0	0	0
PURDUE UNIV	41	56	60	0	75
RICE WILLIAM MARSH UNIV	45	68	109	0	84
STANFORD LELAND JR UNVR	448	287	281	300	415
TEXAS TECH UNIV	7	0	0	0	0
TEXAS UNIV OF	65	84	93	0	100
VIRGINIA POLYTECHNIC INST	0	74	48	51	92
WASHINGTON UNIV OF	0	0	38	40	43
WISCONSIN UNIV OF	0	5	0	0	0
YALE UNIV	32	54	49	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0402020 INFORMATION ANALYSIS TECHNIQUES					
OPERATING EXPENSES					
FLORIDA UNIV OF	49	58	50	0	0
GEORGE WASHINGTON UNIV	0	80	0	0	0
PRINCETON UNIV	116	217	257	0	175
STANFORD LELAND JR UNIV	70	25	0	0	0
UTAH UNIV OF	0	100	120	132	150
WISCONSIN UNIV OF	153	0	95	86	120
KC0402030 ADVANCED COMPUTER SYSTEMS CONCEPTS					
OPERATING EXPENSES					
CALIF UNIV OF LOS ANGELES	250	125	0	0	0
CALIFORNIA INST OF TECH	0	0	550	600	1200
COLORADO UNIV OF	100	99	100	0	100
GEORGE WASHINGTON UNIV	0	0	50	55	60
ILLINOIS UNIV OF	125	138	155	60	500
MASSACHUSETTS INST TECH	250	314	100	195	625
NEW YORK UNIV	250	500	600	630	850
TEXAS UNIV OF	98	100	107	0	500
WISCONSIN UNIV OF	0	0	8	0	0
KC0402040 SPECIAL PROJECTS					
OPERATING EXPENSES					
NEW YORK UNIV	50	100	100	150	150

9. **The budget justification (Congressional Budget Request, FY 1985, Volume 3, p. 167) notes that the "subactivity in Advanced Computing Concepts will be expanded with an increment of $3,230,000 in order to provide additional research staff, graduate students, and engineering support for research mechanisms being investigated at universities and laboratories that have demonstrated viable designs for novel architectures." Who are these universities and laboratories referred to, and how are these incremental funds expected to be distributed?**

Answer: Projects in Advanced Computing Concepts and their funding levels for FY 1984 and the amounts which have been formerly requested by each institution in FY 1985 are as follows:

Site	Investigator	FY 1984 Funding	FY 1985 President's Budget	Increment
Cal Tech	Fox, Seitz	$ 900,000	$1,200,000	$+ 300,000
MIT	Dennis	231,000	500,000	+ 269,000
MIT	Fredkin	110,000	125,000	+ 15,000
NYU	Lax, Kalos	630,000	850,000	+ 220,000
Illinois	Kuck, Lawrie	226,000	500,000	+ 274,000
Texas	Browne, Kipsovsky	159,000	500,000	+ 341,000
Argonne	Messina	1,189,000	1,550,000	+ 361,000
LANL	Buzbee	700,000	1,300,000	+ 600,000
LBL	Quong	200,000	900,000	+ 700,000
LLNL	Michael	500,000	650,000	+ 150,000

10. **The budget justification also states that one state-of-the-art supercomputer will be leased in FY 1985 to satisfy the computing requirements of the Energy Research programs. What type of computer will be leased?**

Answer: Our plan is to lease an enhanced Class VI computer to expand the capacity at the Magnetic Fusion Energy Computer Center (MFECC) at the Lawrence Livermore National Laboratory to satisfy the large scale scientific computing needs of the Energy Sciences Programs. Expansion of the MFECC network to accommodate the Energy Sciences represents the lowest cost alternative for providing these programs with high quality supercomputer service in the shortest time.

11. **What cooperative projects among university, DOE laboratory, and industry supercomputer researchers are currently underway? What such projects are envisioned for the remainder of FY 1984 and FY 1985?**

Answer: In FY 1984 cooperative projects are underway between Cal Tech and Intel, New York University and IBM, Argonne and Denelcor, Los Alamos and Denelcor, Lawrence Berkeley and Digital Equipment Corporation (DEC), and Lawrence Livermore and DEC. These projects are detailed below.

The Cal Tech-Intel project, "Concurrent Processing and the Decomposition of Problems" involves the design and implementation of a homogeneous architecture machine called the Cosmic Cube.

The NYU-IBM project, "Ultracomputer," involves the design and implementation of a 512 processor ultracomputer with the NYU replace-add omega network.

The LLNL-DEC and LBL-DEC projects involve algorithm development on the DEC MPVAX, a four processor Vax 11/780 machine. There is an agreement to replace this with a 64 processor micro-Vax machine when it becomes available.

The LANL-Denelcor and ANL-Denelcor projects involve algorithm development for the Denelcor HEP-1 machine. LANL is concentrating on numerical algorithms for partial differential equations and ANL is investigating logic programming and robust mathematical software. The HEP-1 has an interesting pipeline architecture that makes parallelization of algorithms relatively straightforward.

For the remainder of FY 1984 and in FY 1985 these projects will continue and, in some cases, grow substantially. Potential new projects include participation by the University of Illinois, MIT, Princeton, UC Berkeley, University of Texas, Yale, Purdue, Florida State and others, each with industrial partners. The final allocation of FY 1985 funds will be based on peer review of unsolicited proposals.

12. **Five percent of the Class VI computer time on the Magnetic Fusion Energy network was made available to other Energy Research programs beginning in May 1983. How much computer time was made available, and how much computer time was requested by researchers?**

Answer: Assuming a nominal availability of 8000 hours per year per machine, 5% of the two Cray-1 computers at the MFECC provides 800 hours per year - thus 300 hours for the last quarter of FY 1983 and 800 hours in FY 1984 are being provided to Energy Research programs outside the MFE program. Proposals received from Energy Research contractors requested more than 10,000 hours of Class VI computer time for projects judged to be appropriate by program managers. These proposals covered work in FY 1983 and FY 1984.

13. **How was the available Class VI computer time allocated? How was the scientific merit of the proposed usage of computer time judged?**

Answer: The available time was allocated to the programs based on the demand indicated by the acceptable proposals received from ER contractors. One half the time went to Basic Energy Sciences, one third to High Energy and Nuclear Physics, and one sixth to Biological and Environmental Research. The proposals from the DOE laboratories were coordinated by laboratory personnel before submission to the appropriate research program managers in DOE. Proposals from university and industry researchers were sent directly to the program managers. Each proposal was reviewed by the cognizant program manager and those found acceptable were ranked by scientific quality and program relevance. Time was allocated on the basis of the probability of getting useful work done with the limited amount of resources available.

14. **How much Class VI computer time has been requested to date by energy researchers in (a) Materials Sciences, (b) Chemical Sciences, (c) Nuclear Sciences, (d) Engineering Research, (e) Geosciences, (f) Applied Mathematical Sciences, (g) Advanced Energy Projects, (h) Biological Energy Research, (i) Nuclear Physics, and (j) High Energy Physics? How much time has been allocated to each of these areas?**

Answer: These figures are displayed in the attached table. This table represents the results of the first set of proposals deemed acceptable by the program managers. The requested hours do not include those deemed not acceptable.

Proposals for Class VI Computing Time for Office of Energy Research Contractors

Discipline	Number Received	FY83 Request (cpu hours)	FY84 Request (cpu hours)	FY 83 Grants (cpu hours)	Number Grants
High Energy Physics	21	1178	3814	72	11
Nuclear Physics	18	413	627	28	5
Subtotal HENP	39	1591	4441	100	16
Materials Sciences	36	1412	2807	68	11
Chemical Sciences	29	512	1161	49	7
Mathematical Sciences	16	469	733	18	4
Engineering Sciences	6	81	125	8	4
Geosciences	9	94	121	7	3
CO2 Climate Research	4	171	183	5	1
Subtotal OBES	100	2739	5130	155	30
Biological Sciences	5	121	160	14	4
Ecological Sciences	6	53	70	14	2
Biophysics/chemistry	12	211	300	17	5
Subtotal OHER	23	385	530	45	11
Total OER	162	4715	10101	300	57

(Note: The number of proposals received does not include multiple proposals received from a single investigator. The total number is close to 200.)

15. **In the past, researchers at laboratories with supercomputers supported by Defense Programs (e.g., Sandia National Laboratories) have been able to obtain supercomputer access for projects supported by Energy Research at no extra charge. Are these researchers being "taxed" or will they be "taxed" to support the Class VI initiative even though they do not require access, and if so, what is the rationale?**

Answer: DOE policies do not provide that any DOE program should get a free ride for computer services. In accordance with OMB Circular A-121, entitled "Cost Accounting, Cost Recovery, and Interagency Sharing of Data Processing Facilities," the Department has established internal policies in DOE Order 2100.8. These policies provide that all Department programs pay their fair share of the costs of the operation of computer facilities commensurate with the amount of resources used. Projects supported by Energy Research therefore should not in fact be getting computer time at no extra charge. The establishment of an ER supercomputing facility is a line item in the FY 1985 budget, just as is the Magnetic Fusion Energy Computing Network. No researchers will be "taxed" to provide access to a facility they do not require.

16. **How does the research funded by the Applied Mathematical Sciences subprogram differ, complement, supplement, or overlap research funded by other DOE programs and by other agencies such as the National Science Foundation or the Office of Naval Research?**

Answer: The research funded by the DOE Applied Mathematical Sciences subprogram supports applied mathematicians and computational scientists at DOE laboratories, universities, and industry working on problems basic to the analysis, development, and use of large scale computational models important in the design of future energy systems. Similarly, the DOD agencies and NASA have a mission orientation to their basic research programs. In some cases, research groups at DOE laboratories and universities are jointly funded to work on fundamental problems of interest to two or more agencies. For example, the difficult problems in inverse scattering theory apply to seismic exploration, nondestructive evaluation of materials, and sonar detection; the applied mathematics group at Ames Laboratory, Iowa State University, is jointly funded by DOE and ONR in a collaborative effort to understand the nature of these problems. Coordination of these efforts is done through frequent personal contact between program managers in the Government and the investigators in the field to ensure that the research is complementary and appropriate for both agencies. Acknowledgment of joint funding is required on all publications produced by such a research project.

In the DOE laboratories, applied mathematicians and computer scientists supported by the AMS program have frequent and useful contacts with the scientists working on problems for other DOE programs. Seminars, workshops, and conferences bring the researchers together with the programmatic scientists to share insight into current problems and advances in the field.

17. What types of formal and informal advisory groups are employed to assure that the subprogram is of high quality and coordinated with the research carried out at other agencies and within other parts of DOE? If any formal advisory groups exist, please provide a listing of the current membership.

Answer: The main "semi-formal" coordinating group for this activity is the Interagency Committee on Extramural Mathematics Programs (ICEMAP). This group has been around for several years, but in the last three years it has become active on a regular basis. Agency members include representatives from the Department of Energy, the National Science Foundation, the Air Force Office of Scientific Research, the Office of Naval Research, the Army Research Office, the National Aeronautics and Space Administration, and the National Bureau of Standards. Occasionally representatives from the National Security Agency, the Central Intelligence Agency, and the National Institutes of Health participate. Special studies on the quality and comprehensiveness of the Federal Government's research programs have been undertaken by several committees of the National Academy of Sciences/ National Research Council, including the Committee on Applied Mathematics, the Committee on Resources in Mathematics, and the Computer Science and Technology Board (for membership lists see NAS/NAE/IOM/NRC publication "Organization and Members, 1981 1982").

Interagency coordination activities are currently being arranged by the Federal Coordinating Council on Science, Engineering, and Technology (FCCSET). FCCSET groups on supercomputer acquisition and access have produced reports this year. An ongoing FCCSET group addressing research in fifth generation computing is active.

18. Please provide a copy of the latest Applied Mathematical Sciences research summaries.

Answer: The booklet "Summaries of the FY 1983 Applied Mathematical Sciences Research Program" is attached.

DOE/ER-0157/1
Dist. Category UC-32

Summaries of the FY 1983 Applied Mathematical Sciences Research Program

December 1983

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering, Mathematical and Geosciences
Washington, D.C. 20545

Table of Contents

Introduction....2
Program Overview....3
Ames Laboratory (Corones)....8
Argonne National Laboratory (Messina)....9
Atlanta University (Mickens)....12
Brookhaven National Laboratory (Peierls)....13
California Institute of Technology (Fox, Seitz)....15
California Institute of Technology (Keller, Saffman)....16
Clarkson University (Bountis)....17
Cornell University (Coleman)....18
Cornell University (Feigenbaum, Siggia)....19
George Washington University (Foley)....20
Indiana University (Foias)....21
Kent State University (Varga, Wang)....22
La Jolla Institute (Tabor, Weiss)....23
Los Alamos National Laboratory (Buzbee, Nichols)....24
Lawrence Berkeley Laboratory (Quong, Concus)....26
Lawrence Livermore National Laboratory (Michael, Carlson)....30
Massachusetts Institute of Technology (Dennis)....33
Massachusetts Institute of Technology (Fredkin)....34
Northwestern University (Matkowsky)....35
New York University- Courant Institute (Lax, Schwartz)....36
Oak Ridge National Laboratory (Ward)....50
Pacific Northwest Laboratory - Battelle (Hall, Erickson)....53
Princeton University (Tukey)....54
Purdue University (Rice)....55
Rice University (Tapia, Dennis)....56
Science Applications, Inc. (Gelinas)....57
Sandia National Laboratories, Albuquerque (Shampine)....58
Sandia National Laboratories, Livermore (Kee)....59
Stanford University (Dantzig, Cottle, Murray)....60
Stanford University (Golub)....61
University of California, Berkeley (Fateman, Kahan)....62
University of California, Berkeley (Marsden, Weinstein)....63
University of Colorado (Fosdick, Osterweil)....64
University of Delaware (Gilbert)....65
University of Florida (Su, Batory, Navathe)....66
University of Illinois (Gear, Watanabe)....67
University of Illinois (Kuck, Lawrie)....68
University of Maryland (Ott, Yorke)....69
University of Texas (Browne, Lipovski, Malek)....70
University of Texas (Carey, Young)....71
University of Utah (Barnhill)....72
University of Washington (Kevorkian)....73
University of Wisconsin (DeWitt, Bates)....74
Virginia Polytechnic Institute (Greenberg, Zweifel)....75
Yale University (Chan)....76

INTRODUCTION

The purpose of this report is to provide a convenient compilation of summaries of the individual research projects that constitute the Applied Mathematical Sciences program in the Office of Basic Energy Sciences, Office of Energy Research, Department of Energy.

The report is ordered alphabetically by institution. DOE laboratories are integrated in alphabetical order with university and other non-DOE institutional participants in the program.

In sequence, each project entry begins with an underlined identification number, followed by the project title, the FY 1983 funds allocated, and the program component identification number:

01 Analytic and Numerical Methods
Includes, Applied Analysis, Computational Mathematics, and Numerical Methods for the Solution of Partial Differential Equations;

02 Information Analysis Techniques
Includes Statistical Methods, Data Management Techniques, and Display and Analysis Techniques;

03 Advanced Computing Concepts
Includes Software Engineering, Distributed Systems, and High Performance Systems;

04 Special Projects
Includes operating and maintenance of Research Computing Facilities and workshops and studies.

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Applied Mathematical Sciences
Division of Engineering,
Mathematical and Geosciences
Office of Basic Energy Sciences
Office of Energy Research
Department of Energy
Washington, D. C. 20545

40-574 O - 85 - 24

U. S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering, Mathematical and Geosciences
APPLIED MATHEMATICAL SCIENCES

Program Overview

Applied Mathematical Sciences serves as the DOE focal point for monitoring and advancing the state of the art in mathematics, statistics, and computer science. Several DOE mission programs develop and refine specific techniques from the applied mathematical sciences applicable to their immediate needs. In contrast, Applied Mathematical Sciences concentrates on more broadly based, continuing needs throughout the DOE community. Emphasis is placed on research basic to the analysis, development, and use of large-scale computational models; the management and analysis of large, complex collections of information; and the effective use of DOE computing resources. The purpose of this research is not to improve existing technologies and methodologies, but rather to render them obsolete.

Each part of the Applied Mathematical Sciences activity has been designed with the help and advice of leading mathematicians and computer scientists from universities, industry, and DOE laboratories to assure the broadest and greatest impact on the nation's energy R&D enterprise. Many of them are expert in industry's needs in the relevant areas. Close liaison is maintained with other Federal agencies in the selection of areas of emphasis and of individual research tasks. This is high leverage research. In favorable cases, the results may be of great benefit simultaneously to a number of different energy technologies.

The FY 1983 budget for Applied Mathematical Sciences is $13,850,000, a $2,250,000 increase over the amount appropriated in FY 1982. Corresponding to the above areas of emphasis, the Applied Mathematical Sciences research program has been organized into four subactivities: Analytical and Numerical Methods, Information Analysis Techniques, Advanced Computer Concepts, and Special Projects.

Analytical and Numerical Methods

In FY 1983, $6,800,000 was allocated for Analytical and Numerical Methods. This research addresses questions basic to improved predictions of the feasibility, reliability, safety, and efficiency of energy systems. Equally important, this research addresses questions basic to the fundamental laws of physics describing the structure and properties of matter, focusing on mathematical and computational techniques. Analytical and Numerical Methods comprises three categories of research activities reflecting the principal thrust of the program in previous years: Applied Analysis, Computational Mathematics, and Numerical Methods for Partial DifferentialEquations.

Applied Analysis research concentrates on techniques to develop and analyze mathematical models of scientific and engineering phenomena. It also includes the analysis of the transition from a mathematical model to corresponding approximate computational models. Subtopics of applied analysis are constructive analysis (model definition), qualitative analysis (existence, uniqueness proofs), quantitative analysis (asymptotics, perturbation), and nonlinear dynamical systems. The latter subtopic deals with the mathematical analysis of turbulence and transition to chaotic regimes.

Computational Mathematics involves the design and analysis of algorithms for basic computational problems (e.g., linear algebra, optimization, approximation and interpolation, and differential equations). Emphasis is placed on the implementation of the resulting algorithms in transportable, high-quality software suitable for software libraries.

Subtopics of computational mathematics are numerical linear algebra (sparse matrices), ordinary differential equations (stiffness, multirate), approximation (interpolation, extrapolation) and optimization (quasi-Newton techniques, mathematical programming).

Numerical Methods for Partial Differential Equations play a dominant role in the modeling of energy systems; access to supercomputers and collaboration with teams of scientists or engineers are usually necessary to develop techniques that ultimately can be used in realistic DOE problems. Currently, this category emphasizes methods applicable to computational fluid dynamics. Subtopics of numerical methods for partial differential equations are multigrid methods (adaptive grid, moving finite elements), continuation methods, discretizations methods, splitting techniques, and Monte Carlo methods.

Although activities in Analytical and Numerical Methods are frequently pursued in collaboration with DOE mission programs (e.g, computer simulation of the combustion of fossil fuels), the research described here is definitely not intended to produce computer models. Rather it yields methodology and tools that can be used by DOE scientists and engineers to construct their models of specific phenomena. The principal objective is to develop methodology and tools applicable to currently intractable problems.

Information Analysis Techniques

In FY 1983, $2,100,000 was allocated for Information Analysis Techniques, which seeks innovative approaches to the manipulation and analysis of large, complex collections of scientific, engineering, environmental, and energy-related data. This activity is organized into three categories: Statistical Methods, Data Management, and Display and Analysis Systems.

Statistical Methods addresses issues fundamental to analyzing both the input and the output of data intensive studies. Subtopics are exploratory data analysis, computational statistics, and sensitivity analysis applicable to large, complex data collections and multi-parameter

models, where traditional statistical methods have proven inadequate.

Data Management encompasses computer science research underlying the organization and retrieval of large, complex data collections. Currently, the interface with interactive display and analysis of numerical data is emphasized; plans include the interface with computational models and new projects on the design of database machines for very large scientific and engineering data sets.

Display and Analysis Systems studies methods for making graphics, data management, and analysis tools more unified and easier to use. These efforts are studying techniques for displaying multidimensional sets representing large experimental data sets and the output of complex analytical models of combustion processes. Subtopics are projection pursuit techniques, multidimensional surface interpolation, and advanced graphical display techniques.

Advanced Computing Concepts

In FY 1983, $4,285,000 was allocated for research in Advanced Computing Concepts, an activity that is based upon three premises: 1) the computer industry will continue to improve cost-performance ratios for hardware, 2) hardware systems will increasingly be tailored to specific classes of applications, and 3) the cost of software development and maintenance will dominate all other computing costs. Based upon these premises, three categories of Advanced Computer Concepts are distinguished: Software Engineering, Distributed Systems, and High Performance Systems.

Software Engineering includes research on programming languages and automated programming aids, with emphasis on ultimate applicability to large-scale computational models. Software Engineering research activities seek a better understanding of the process of creating transportable, high-quality software implementations of algorithms for basic computational problems, the building blocks of computational models, and therefore interacts strongly with Computational Mathematics. Emphasis in placed on applicative languages, program transformation and automated reasoning techniques, and design of tools for integrating symbolic and numerical programming techniques.

Distributed Systems includes research on both local and remote networks. Research on local networks emphasizes performance of links between worker computers (e.g., supercomputers), mass-storage systems, and interactive access. Research on remote networks addresses the problem of resource utilization in a heterogeneous environment (e.g., program development on a highly interactive system with automated programming aids, program execution on a supercomputer, and analysis of results on an interactive graphics facility).

Current work is aimed at developing interprocess communication primitives that will allow heterogeneous computer networks to behave as a single, integrated computational resource.

High Performance Systems research activities respond to the fact that computer hardware development has reached a fundamental limit imposed by finite signal propagation speeds. While new technologies may alleviate heat generation in circuitry and therefore permit more compact and thus faster systems, increased computing power will ultimately depend upon parallel execution of instructions. High Performance Systems, therefore, emphasizes two critical areas: the match between algorithmic structure of large-scale computational models and the possible architectural structure of future supercomputers, and the transportability of applications software between successive generations of supercomputers. The topic does not include areas covered by the DOD's VLSI and VHSIC programs; nor does it apply to high speed image processing or signal processing applications. The major focus is on large scale scientific computing and the parallel architectures and concurrent algorithms necessary for long range research in the computational sciences. This includes the design and construction of engineering prototypes for several experimental parallel architecture machines. Research in algorithms, languages, and operating systems for parallel architectures in the fastest growing area of the Applied Mathematical Sciences research program.

Special Projects

In FY 1983, $665,000 was allocated for Special Projects to support conferences and working groups to evaluate program directions, operation and maintenance of the Research Computing Facilities, and selected special projects outside the previously defined topic areas. Examples of these activities include a High Speed Computer Workshop sponsored by LLNL and LANL that includes representatives from all the major mainframe manufacturers and scientists from the DOE community, a symposium at LANL's Center for Non-Linear Studies, and several visiting scientist programs that serve to bring distinguished visitors from the universities to the national laboratories.

Capital Equipment
Research Computing Facilities in the Applied Mathematical Sciences Program

In FY 1983 $800,000 was allocated for capital equipment in Applied Mathematical Sciences for the DOE Laboratories and the Courant Institute for Mathematical Sciences at New York University. Equipment funds for other university programs do not come from this budget - rather, funds for university equipment is allocated out of the operating funds budget and title is, therefore, usually vested in the university. The Applied Mathematical Sciences (AMS) research program is supporting the development and operation of Reseach Computing Facilities (RCF's) at several DOE National Laboratories and universities. Each RCF will consist of one or more minicomputers dedicated primarily to a specific thrust of the AMS research program. Although the principal users of an RCF will be the staff at the host site, each RCF will be available as a resource for other AMS researchers participating in the associated thrust area. The RCF's will be linked by one or more existing computer networks to:

a. facilitate access by researchers without a local RCF;

b. stimulate interactions among various AMS supported research groups; and

c. provide a resource for research on distributed systems.

Where appropriate, an RCF will be linked to the Central Computing Facility of the site. Thus, the RCF's will also serve as gateways to large-scale scientific computers and other DOE computing resources.

The Research Computing Facilities provide mathematicians, statisticians, and computer scientists with the resources to explore innovative new approaches to utilizing the developments of computer technology, while simultaneously developing new technological frontiers. While other scientists and engineers use the computer as a tool to simulate and analyze experiments, the computer research community uses the computer itself as the object of experimentation. This experimentation is obviously incompatible with the stability of the computing environment required to serve the computing needs of other disciplines. Essentially all FY 1983 Capital Equipment funds were allocated to these Research Computing Facilities.

The acquisition of most parts of the RCF network is nearing completion, after nearly five years. As such it represents the only "integrated" setup in the United States, in which applied mathematicians, statisticians, and computer scientists from universities, government laboratories, and industry can collaborate directly on a daily basis from all over the country.

DOE Applied Mathematical Sciences FY 1983

AMES LABORATORY
Department of Mathematics and
Applied Mathematical Sciences
Iowa State University
Ames, Iowa 50011

01. ANALYTICAL AND NUMERICAL METHODS $300,000 01
$25,000 Eqmt

James Corones, B. Carlson, M. Davison,
A. K. Gautesen, H. McMaken, R. Krueger

Applied Analysis

The work being done is exclusively in the area of applied analysis. The effort is focused on basic and applied problems in linear and nonlinear wave propagation. In the area of linear wave propagation, particular attention is given to direct and inverse scattering theory and related areas, e. g., tomography. The purpose of this work is to develop mathematical procedures and tools that can be used to characterize and/or image nonuniformities in materials (density variations, stress fields, cracks, potential, for example). Two types of approaches are pursued: 1) direct scattering, in which the nonuniformities are given and the objective is to compute the scattered field, e. g., of elastic waves scattered by cracks, and thereby determine characteristic signatures of scatterers; and 2) inversion procedures, in which incoming and outgoing signals are assumed known and the objective is to deduce the nonuniformities from this knowledge, e. g., mapping density variations using x-ray tomography. Inversion studies attempt to incorporate realistic constraints such as limited angles of view, limited apertures and noise. The techniques developed have wide application, including quantitative NDE, geoprospecting, remote sensing of nuclear waste, plasma diagnostics, and fission reactor diagnostics. At present, QNDE is the major applications orientation of the effort. There is a modest effort in nonlinear wave propagation focused on the study of equations that support soliton solutions. In addition, work on special functions directed at facilitating their use and computation is carried out.

DOE Applied Mathematical Sciences FY 1983

ARGONNE NATIONAL LABORATORY
Mathematics and Computer Science Division
9700 South Cass Avenue
Argonne, Illinois 60439

02. ANALYTICAL AND NUMERICAL METHODS $850,000 01

P. C. Messina,
H. G. Kaper, G. K. Leaf,
B. J. Matkowsky, A. Zettl
W. J. Cody, Jr., J. J. Dongarra,
B. S. Garbow, K. E. Hillstrom,
J. N. Lyness, M. Minkoff,
J. J. More', D. C. Sorensen

This task consists of research in the areas of applied analysis and computational mathematics. Current interest in applied analysis centers on the modeling and analysis of reaction-diffusion systems, bifurcation phenomena in combustion problems, and fluid flow problems related to loss-of-coolant analysis in reactor engineering. While specific areas of investigation may vary in response to changing DOE needs, the long-term objectives remain the same: the mathematical modeling of observable phenomena, the analysis of the mathematical model, and the interpretation of the analytical results. The computational mathematics research involves the design and analysis of numerical algorithms, the development of special techniques to measure algorithm reliability and efficiency, and the preparation of software based on broadly applicable computational methods. Efforts focus on development of new algorithms for special and elementary functions; investigation of optimization algorithms; design and dissemination of quadrature techniques; study of methods for solving partial differential equations; and development of improved techniques for solving problems in numerical linear algebra, including algorithms for vector pipeline and parallel computers. In addition, work on software evaluation has been renewed, and special methods are being developed for use in chemical equilibrium problems.

ARGONNE NATIONAL LABORATORY
Mathematics and Computer Science Division
9700 South Cass Avenue
Argonne, Illinois 60439

03. ADVANCED COMPUTER CONCEPTS $1,050,000 03
P. C. Messina,
J. M. Boyle, W. J. Cody, Jr.,
W. R. Cowell, J. J. Dongarra,
K. W. Dritz, J. R. Gabriel,
B. S. Garbow, K. E. Hillstrom,
E. Lusk, R. Overbeek
B. T. Smith, L. T. Wos

This task consists of research in the area of software engineering. The objective is to develop new techniques for designing and producing highly reliable, easily usable computer software. Particular attention is given to studies in automated reasoning, including formulation of new strategies and inference rules for our theorem provers and design of an abstract architecture for automated deduction systems. Other activities include work on abstract programming and program transformation, as well as language-related studies on extensions to Fortran and PL/I and coordination of a multi-institutional project to produce tools for numerically oriented software.

DOE Applied Mathematical Sciences FY 1983

ARGONNE NATIONAL LABORATORY
Mathematics and Computer Science Division
9700 South Cass Avenue
Argonne, Illinois 60439

04.	SPECIAL PROJECTS/	$100,000	04
	RESEARCH COMPUTING FACILITY	$150,000	Eqmt
	P. C. Messina,		
	J. M. Boyle		

This special project involves the development and operation of a Research Computing Facility (RCF). The facility provides an opportunity to explore the effectiveness of using smaller computers for mathematical software research and for collaborative studies among AMS-funded groups. The RCF is currently based on a Digital Equipment Corporation VAX 11/780 computer. Experiments on the RCF continue in computational mathematics, automated reasoning, and on the TAMPR transformation program.

ATLANTA UNIVERSITY
Department of Physics
223 Chestnut Street, SW
Atlanta, GA 30314

05. ANALYTICAL AND NUMERICAL METHODS $62,000 01
Ronald E. Mickens

Investigation of Perturbation Techniques for Nonlinear Difference Equations and Related Problems

Our major research activity will be the construction of a number of regular and singular perturbation techniques that may be used to obtain approximate analytical solutions to several classes of nonlinear difference equations. Emphasis will be on those procedures that lead to uniformly valid asymptotic solutions. An investigation will be carried out on the modeling of nonlinear, first order ordinary differential equations by difference equations. In particular, procedures that give rise to models with zero local truncation error will be emphasized.

Results expected from this work include the following possibilities:

1. The construction of both singular and regular perturbation techniques for classes of nonlinear ordinary and partial difference equations that are used in nonlinear heat, wave, and field theories;

2. A possible solution to the problem of spurious solitons that arise in difference equation modeling of continuum field theory and solid state physics;

3. A set of rules for constructing difference equation models of first order ordinary differential equations with no local truncation error in the numerical solutions;

4. Rules that eliminate the multiplicity of solutions to finite difference approximations of differential equations; and

5. Perturbation techniques for investigating finite amplitude instabilities of partial difference equation models of physical phenomena.

This project is a new start in FY 1983.

BROOKHAVEN NATIONAL LABORATORY
Applied Mathematics Department
Upton, New York 11973

06. ANALYTICAL AND NUMERICAL METHODS $325,000 01
C. Goldstein, H. Stewart, J. Pasciak, R.Marr

Analytical and Numerical Methods

The emphasis of this research is the extension to new domains of existing methods for modeling important physical phenomena and the development of new methods especially for intrinsically three dimensional problems. Finite element methods for problems involving unbounded domains previously developed were investigated. A hitherto unrecognized shortcoming in the error analysis of numerical solutions of the wave equation was discovered and a correct treatment implemented. A recently developed method for the solution of magnetostatic field problems was completed for an important class of three dimensional problems. Further work on numerical methods for approximating steady state harmonic eddy currents was carried out. Nonlinear oscillator models applicable to a wide range of physical, chemical, and biological systems were being studied. Computer animation techniques for generating phase space portraits of dynamical systems were refined and applied to a number of problems. Extensions to existing NMR imaging schemes were investigated including techniques for faster acquisition of full 3D images. A new approach to spatially mapping NMR frequency spectra was implemented. Preliminary applications of this approach to simple simulated data have been carried out.

DOE Applied Mathematical Sciences FY 1983

BROOKHAVEN NATIONAL LABORATORY
Applied Mathematics Department
Upton, New York 11973

07. INFORMATION ANALYSIS TECHNIQUES $275,000 02
C. S. Kao, H. Robbins, J. van Ryzin, R. Peierls, W-Y. Tsai

Statistical Methods

This task is concerned with developing and studying improved statistical methods for Survival, Risk, and Reliability problems, which deal with questions about when and whether a set of specified subjects will experience some undesirable event. The death of human beings from specific causes and the failure of complex machinery are examples. Studies are concerned with the censoring effects of finite duration or of competing causes, as well as with the need to extrapolate. In FY83 several results were obtained that improved on previous estimation techniques for censored data. Empirical Bayes methods apply to observations drawn independently from a family of distributions. While conventional methods estimate each independent distribution on the basis of its own set of observations, Empirical Bayes approaches the problem globally using simultaneous inference on all. Reliability of estimates can be significantly improved. In FY83 results on simultaneous variance estimation were improved. Sequential methods use the results of observations to date in a study to affect the choice of which observation to take next or whether to stop. They are important in investigations where the observations are difficult, costly, or have undesirable side effects. In FY83 a sequential algorithm for optimal estimation of a linear combination of means using a fixed total number of observations was implemented and tested for a variety of model problems. Work on reliability estimation for structures in the presence of randomly combined loads was continued.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Division of Physics, Mathematics and Astronomy
Division of Engineering and Applied Science
Pasadena, California 91125

08. ADVANCED COMPUTING TECHNIQUES $550,000 03
Geoffrey C. Fox, Charles L. Seitz, Co-Principal Investigators
H. Keller, P. Saffman, Applied Mathematics
R. Bryant, A. Martin, Computer Science
R. Clayton, B. Hager, Geophysics
A. Kuppermann, Chemistry
M. Salama, Applied Mechanics, JPL

Concurrent Processing and the Decomposition of Problems

This project establishes an interdisciplinary research group in concurrent computation. The research covers the construction of a homogeneous architecture machine with up to 1024 nodes and the appropriate system software as well as the development of algorithms and software for many different applications. The group has a strong technical base with scientists in computer science and applied mathematics. The group will initially cover the areas of high energy physics, geophysics, chemistry, and applied mechanics with scientists who are leaders in their respective fields. It is anticipated that this group will play a major role as a focus and catalyst for the revolution in scientific computing that will be caused by the replacement of conventional computers by concurrent processors. The project provides for substantial involvement by scientists outside Caltech. The intent is to abstract the general features of the concurrent decomposition of problems and use these as the design criteria for future machines and the basis for algorithms in new applications.

This project is a new start in FY 1983.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Department of Applied Mathematics
Pasadena, California 91125

09. ANALYTICAL AND NUMERICAL METHODS $248,847 01
H. B. Keller, P. G. Saffman

Numerical Analysis, Scientific Computing, and Fundamental Studies in Fluid Mechanics

This project is a broad program on problems directly related to energy research and to the methods by which they are solved by means of scientific computing. The program has three distinct but interrelated aspects:

1. Investigation of specific phenomena and/or problems related to energy research (basically in fluid mechanics);

2. Development of numerical methods and algorithms for the solution of problems or the simulation of phenomena;

3. Development of software, graphics, networking and special devices to aid scientific computing.

The main physical phenomena under study center on steady incompressible flows, both viscous and inviscid - including transition to turbulence, vortex dynamics, flow in porous media, structure and stability of vortical states, and a variety of specific steady viscous flows in finite and infinite domains. Some work on seismic ray tracing and geophysical inverse problems has also been included.

The main emphasis on numerical methods development has been in the general area of path following and continuation methods, with particular attention to limit point and bifurcation phenomena. This includes global Newton and homotopy methods. These ideas have been employed along with finite difference and spectral methods for solving two point boundary value problems, partial differential equations and integral equations. Adaptive mesh selection and curvilinear overlapping grid methods have also begun to play a role in this work. Sparse matrix techniques have been studied and efficient algorithms for solving large nonlinear systems have been devised. Numerical methods for conformal mapping are under active development in this program.

DOE Applied Mathematical Sciences FY 1983

CLARKSON COLLEGE OF TECHNOLOGY
Mathematics and Computer Science Department
Potsdam, NY 13676

10. ANALYTICAL AND NUMERICAL METHODS $18,604 01
Tassos Bountis

Stable and Chaotic Dynamical Systems and Their Singularities in the Complex Time Plane

A new and exciting approach in the study of chaos in dynamical systems has been recently proposed in which the principal investigator has been actively involved. According to this approach the main chaotic properties of a dynamical system are determined by the movable (i. e., initial condition dependent) singularities of its solutions in the complex time plane. One of the virtues of the method is that it is direct to the point that it could be solved numerically on a computer.

It is known that if the solutions possess no singularities other than poles the system is completely integrable. Moreover, if besides poles the solutions of a Hamiltonian system also admit logarithmic terms in (t - t0), the motion is still generally stable, while "worse" singularities are connected with large scale chaotic behavior in phase space. The research objectives of this project are:

1. To study the precise qualitative and quantitative relationship between different types of singularities and different chaotic properties of dynamical systems;

2. To analyze the singularities of integrable Hamiltonian systems and examine their effect on the behavior of "nearby" non-integrable Hamiltonians; and

3. To study the location of the singularities as the system undergoes a transition to chaos through a sequence of bifurcations of its main periodic orbits.

This project is a new start in FY 1983.

CORNELL UNIVERSITY
Department of Computer Science
Ithaca, NY 14853

11. ANALYTICAL AND NUMERICAL METHODS $38,866 01
Thomas F. Coleman

Topics in Large Sparse Nonlinear Optimization

Many problems in the physical sciences, engineering, and econometric disciplines involve the numerical solution of a system of nonlinear equations or the computation of the minimizer of a nonlinear function. Often these nonlinear problems are of large dimension involving several hundred to several thousand variables. Typically, the relevant Jacobian and Hessian matrices are sparse (i. e., many zero elements). In addition, it is often the case that a single evaluation of the function or gradient is an expensive operation. The purpose of the proposed research is to explore ways in which sparsity can be exploited so that the number of function (gradient) evaluations is 'minimized' and yet a solution is obtained efficiently. In particular, this project will examine several computational questions concerning the efficient estimation of a sparse symmetric Jacobian matrix by finite differences and the economic use of partial Jacobian information. Several related issues that arise when minimizing a large sparse nonlinear function in the presence of constraint functions will be examined.

This project is a new start in FY 1983.

40-574 O - 85 - 25

DOE Applied Mathematical Sciences FY 1983

CORNELL UNIVERSITY
Laboratory of Atomic and Solid State Physics
Ithaca, NY 14853

12. ANALYTICAL AND NUMERICAL METHODS $127,417 01
Mitchell J. Feigenbaum, Eric D. Siggia

Systems Near the Onset and in the
Well Developed Regimes of Turbulence

This project represents a program of research dedicated to chaotic behavior in both the onset regime and in the fully developed (or high modal) regime. The investigations entail a blend of a computational effort to gain data to support the insights and to assist in the development of a theoretical effort employing recently developed methodologies and ideas.

The first aspect of this program - work pertaining to the onset of turbulence - is founded on the fact that universal minimal (and low) modal models can successfully embrace the behavior of real continuum systems. Our attack includes the investigation of chaos borne from low-order quasiperiodicity; modifications of these phenomena in the presense of spatial symmetries; the continued investigation of functional integrals in order to determine the sensitivity of these processes to external noise and to attempt to develop descriptions of the fractional dimensional attractors that determine post-onset turbulence.

The second aspect of this project is centered on intrinsically high modal turbulence arising either from the onset behavior in large cells or from high Reynolds number excitations. In the first case, we intend to continue investigations of theories to describe pre-Hopf bifurcation drifts in degenerate spatial structures. In the case of fully developed turbulence, we intend to perform investigations of details of the flow that can clarify the role of large scales in determining small scale intermittency.

This project is a new start in FY 1983.

THE GEORGE WASHINGTON UNIVERSITY
Department of Electrical Engineering and Computer Sciences
Washington, D.C. 20052

13. INFORMATION ANALYSIS TECHNIQUES $50,000 03
James D. Foley

Scientific Work Station Research

Object oriented languages provide for the high level manipulation of well defined data structures and operations on these structures, the details of which are hidden from the programmer. High level languages are designed to provide a better quality programming environment, freeing the user from having to understand the details of the underlying architecture and operating system. Object oriented languages are particularly well suited for concurrent processing because parallel activities can be automatically detected and synchronized by the compiler, instead of being explicitly directed by the user.

Graphics programs inherently have a large amount of parallel operations, both in parallel with the applications programs generating the displays and internally within the graphics package, where concurrent frame generation, transformations, and interactive device handling are carried out independently. Thus it is advantageous to be able to express operations in terms of manipulation of objects and have various functions assigned automatically to the appropriate processor for concurrent processing. Due to the usually complex nature of scientific graphics displays, the multiprocessor scientific work station is an ideal setting for the investigation of these techniques.

This research will focus on two areas: the design of an object oriented language that captures the graphics functionality required for scientific applications and implementation techniques for such languages on multiprocessor scientific work stations.

This project is a new start in FY 1983.

DOE Applied Mathematical Sciences FY 1983

INDIANA UNIVERSITY
Department of Mathematics
Bloomington, IN 47405

14. ANALYTICAL AND NUMERICAL METHODS $84,762 01
Ciprian Foias

Criteria for the Reliability of Numerical Approximations to the Solutions of Fluid Flow Problems

The numerical approximation of the solutions of fluid flow models is a difficult problem encountered in many areas of energy research. In all numerical methods implementable on digital computers, the basic question is how to choose the number of elements, N say (Galerkin modes, finite difference cells, finite elements, etc.) in order to guarantee that the approximation at least behaves like the exact solution. In the absence of a rational prescription for the determination of this number until now, it has been estimated either empirically or on the basis of physical intuition. The purpose of the proposed research is to derive useful estimates for N from some newly discovered fundamental properties of the viscous incompressible Navier-Stokes equations.

The proposed research will contribute to the problem of the numerical solution of fluid flow equations. The specific objectives of the proposed research are:

(a) To determine the minimum number of Fourier modes that must be carried in the application of Galerkin's method to the viscous incompressible Navier-Stokes equations in order to guarantee that the approximation behaves like the exact solution with the same initial conditions;

(b) To extend the results of (a) to other methods (finite differences, finite elements, and hybrid methods);

(c) To apply the results of (a) to sample standard problems of hydrodynamics.

Successful completion of the proposed research will be useful in providing rigorous reliability criteria for the numerical approximation of the solutions of a wide class of fluid flow models encountered in many energy related applications. The study of the problems to which the proposed research addresses itself is of great interest in general because it introduces to numerical methods for partial differential equations new and powerful nonlinear methods of analysis.

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Department of Mathematics
Kent, Ohio 44242

15. ANALYTICAL AND NUMERICAL METHODS $199,000 01
R. S. Varga, P. S. Wang

Applications of Numerical Analysis and Computer Symbolic Computation

The major emphasis for this research is on the theoretical basis for workable numerical algorithms for general iterative methods in linear algebra, and for workable algorithms for inclusion in Vaxima. The research areas are:

(1) An analysis of basic iterative methods for matrix equations;

(2) The use of symbolic and numerical techniques to settle the long-standing conjectures of Whittaker (in function theory) and Bernstein (in approximation theory);

(3) The integration of symbolic (exact) and numerical (approximate) computing techniques in the VAXIMA system.

Current emphasis is on the theoretical understanding of matrix factorization, incomplete polynomials, and generalzed Bessel polynomials. Many improvements to the Vaxima system will be made in the area of polynomial factorization algorithms, partial fractions, complex numbers, and Pade' approximates.

LA JOLLA INSTITUTE
Center for Studies of Nonlinear Dynamics
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La Jolla, California 92038

16. ANALYTICAL AND NUMERICAL METHODS $86,252 01
Michael Tabor, John Weiss

Studies of Turbulence in Dynamical Systems

We are applying a numerical method based on Taylor series expansions to uncover the analytic structure (singularities) of several dynamical systems that display "turbulent" behavior. Among these are the Lorenz, Henon-Heiles, and point-vortex systems. Our results show a correlation between the structure of the complex-time singularities and the qualitative properties of the real-time motion.

By considering the detailed properties of the expansion of a solution about a singularity, we have been able to predict, for a given system, the nature of its singular set. Natural boundaries with a "fractal" structure are found for a wide of class of non-integrable dynamical systems. Our analysis agrees well with the structures found numerically. In addition, our results show certain connections between the multivaluedness of a system's singularities and the appearance of chaotic motion. By contrast, the property that the only movable singularities are simple poles (the Painleve' property) enables us to identify parameter values for which a given system is completely integrable.

An analogue of the Painleve' property is also being developed for partial differential equations; this involves an expansion of the solution about its singular manifold. This analysis provides a test of integrability (in any numbers of dimensions) for these systems. In addition, it provides a systematic means of obtaining Backlund transformations, Lax pairs, and special solutions.

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17. ANALYTICAL AND NUMERICAL METHODS $300,000 01
Basil Nichols, Mitchell J. Feigenbaum
Thomas D. Butler, James M. Hyman

Numerical Analysis and Nonlinear Mathematics of Energy Systems

Numerical mathematical models at the heart of current energy research problems involve, in an essential way, the numerical solution of complicated systems of nonlinear partial differential equations. Our project is to unify and simplify new solution algorithms for such systems. Recent developments emphasize adaptive mesh methods such as adaptive multigrid and front tracking to resolve subgrid scale structures of discontinuous solutions. We also are creating software to resolve large nonsymmetric, nonlinear algebraic systems arising on irregular meshes. In multidimensional computational fluid dynamics, this program has partially supported numerical methods development in a particle-fluid model for spray dynamics; a new free Lagrangian computing technique; and in documenting a general code for calculating transient aerodynamics flows.

Jointly with the Center for Nonlinear Studies at Los Alamos, the main thrust of our effort in applied analysis is directed at investigating universality and chaos in dynamical systems. Indeed the role of low dimensional phenomena in determining the behavior of complex physical continua at the onset of turbulence has come to be understood in the last few years. This program has partially supported developments in metric universality properties of low dimensional maps. Transition to turbulence is especially delicate to track in complex reactive flows; a companion effort is aimed at the systematic understanding of the role of complex chemistry in combustion waves, in realistic physico-chemical situations.

DOE Applied Mathematical Sciences FY 1983

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18. ADVANCED COMPUTER CONCEPTS $645,000 03
$90,000 Eqmt

Billy Buzbee, Thomas Jordan,
Paul Frederickson, Robert Hiromoto,
Joseph Fasel, Ingrid Bucher

High Performance Systems

By 1985, vendors of high performance systems may offer multiprocessor systems in which four or more processors share a common memory and collaborate on a common task. Such a system could be used to multiprocess a numerical simulation, but to do so requires revolutionary changes in scientific computing. In particular, we will need algorithms that lend themselves to efficient partitioning across processors and software that facilitates implementation of these algorithms. These are the objectives of Los Alamos' research in high performance systems.

Although multiprocessing is an old idea, there is little experience with it. Thus in addition to developing algorithms, we have set as one of our goals the performance of computational experiments using any suitable equipment. Experiments are necessary to 1) determine if our algorithms work, and 2) if so, how well they work - i.e., obtain quantitative performance data. The latter is particularly important because overall performance of a multiprocessor system is strongly dependent on average utilization of individual processors. Since full scale DOE simulation models often require several person-years of effort to transport from one system to another, our technical approach is to incorporate our algorithms into "benchmark models" that are representative of full scale simulations but of manageable proportions. Benchmark models associated with particle-in-cell calculations, Monte Carlo calculations, and diffusion calculations will be developed and used in our experiments. These three areas encompass a large portion of DOE large scale calculations in energy research and weapon design.

Based on the experience obtained from these experiments, we will explore language constructs for implementing our algorithms.

Included in this project is the operation of an RCF including a Vax on the Arpanet and a Denelcor HEP-1 used as an experimental computer.

DOE Applied Mathematical Sciences FY 1983

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19. ANALYTICAL AND NUMERICAL METHODS $500,000 01
N. Albright, A.J. Chorin, P. Colella, P. Concus, A. Fogelson, F.A. Grunbaum, O.H. Hald, A. Majda, T. Nanda, J.A. Sethian

The Analytical and Numerical Methods program at LBL focuses on the areas of vortex dynamics and turbulence, high resolution methods for hyperbolic equations, reacting flows, capillarity phenomena, inverse problems, numerical solution of elliptic partial differential equations, and the dynamical theory of band matrices. A central goal is the construction of mathematically sound, computationally efficient, and physically realistic models that can lead to fundamental scientific understanding and are capable of being used for engineering purposes. The vortex dynamics and high resolution methods provide powerful and general methods for solving the equations that arise in turbulent flow, multiphase displacement in porous media, and other areas. Coupled with additional techniques they provide an effective basis for attacking problems in reacting flows such as combustion and flame propagation and the adhesion and aggregation of platelets in blood. The other topics of interest provide numerical and mathematical methods for attacking broad classes of problems including free surface problems, the reconstruction of the density of the earth from free oscillation data, the reconstruction of images of objects from projection data of their transverse sections, and the determination of eigenvalues of matrices.

DOE Applied Mathematical Sciences FY 1983

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20. INFORMATION ANALYSIS TECHNIQUES $600,000 02
C. Quong, A. Shoshani,
P. Hawthorn

Research in Information Analysis Techniques seeks innovative approaches to the management, manipulation and display of large, "scientific and statistical data bases" [SSDBs]. Data bases created and collected for scientific, socio-economic, demographic, and similar applications, have requirements that cannot be easily supported by existing commercial data management systems.

The data management research program has three major components that address the specialized problems of SSDBs. In the "user interface" area we are exploring several approaches suitable to users with different needs. The "physical organization" area is concerned with compressing data and accessing them efficiently, as well as managing files on secondary storage. The "modeling" area bridges the user interface and physical organization areas, by dealing with models of both logical and physical data structures. These models allow multiple user interfaces to co-exist in a single system, and provide the basis for query optimization and processing. In addition, the design requirements of multiple microprocessors to achieve parallel access of compressed and partitioned data has been explored.

DOE Applied Mathematical Sciences FY 1983

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21. ADVANCED COMPUTER CONCEPTS $300,000 03
J. Sventek, W. Greiman
M. O'Dell

The Advanced Computer Concepts program has concentrated on research problems in the effective use of distributed computer systems. A major thrust of the distributed systems research program is the performance measurement of local-area network interconnection hardware, performance measurement of communication protocol implementations utilizing this hardware, and subsequent analysis of the measurements using simulation and other modelling techniques. As a result of this work, realistic estimates of local-area network performance in DOE environments can be made; additionally, the enhancements to network hardware and software necessary to achieve required performance characteristics can be determined.

A second facet of the research program concerns design methodologies for distributed applications. The activities in this area are concerned with communication protocol design, with special emphasis on methods to simplify such designs for application programmers. Important issues in this work are 1) ease of use of the resulting protocol, 2) reliance of the protocol on generic services provided by lower-level protocols, rather than exploiting the features of one specific support protocol, and 3) providing location transparency of network objects. Such studies are especially important, since they are crucial to the effective utilization of the many heterogeneous network configurations found in the DOE computational community.

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22.	SPECIAL PROJECTS/	$100,000	04
	RESEARCH COMPUTING FACILITY	$100,000	Eqmt
	C. Quong		

The Research Computing Facility (RCF) provides the computational resources needed to support the ongoing basic research in Applied Mathematical Sciences. It serves as a testbed for the evaluation and deployment of new computing capabilities as well as serving as the hub of the Electronic Mail System. Maintenance and development of the RCF, including integration and evaluation of emerging computing technologies, is a focal point for collaborative interaction with other DOE research sites and with researchers in computer science throughout the university and industrial communities.

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23. ANALYTICAL AND NUMERICAL METHODS $175,000 01
George Michael, Ralph Carlson,
Fred Fritsch, Alan Hindmarsh

Computational Mathematics

This is one of three DoE, OBES-funded project areas at LLNL, within the overall goal of developing more effective high-speed, large-scale computational capabilities. The goal of the computational mathematics effort is to improve computational speed, accuracy, and effectiveness of high-speed, large-scale computational capabilities. Specific areas of concentration include ordinary differential equation initial value problems, interpolation, and approximation.

In ODE's algorithms and software for the systematized collection ODEPACK were developed further. Two new algorithms were developed for linearly implicit ODE systems, as needed for PDE applications - one for block-tridiagonal coupling (jointly with C. Kenney), and one for general sparse coupling (jointly with S. Balsdon). A study (with P. Brown) of a matrix-free iteration method for stiff systems was begun; speed ups over the standard integrator LSODE, of factors of up to thirty have been observed.

Work continued on the development of physically reasonable, accurate interpolation and approximation algorithms and software. The monotone piecewise bicubic interpolation algorithm first developed last year has been significantly improved. The paper which described the original algorithm has been rewritten to reflect the changes. Software implementing the new algorithm is nearly complete and should be available for distribution in FY84. A report describing the software is currently in preparation. Several new multi-stage interpolation algorithms for solving scattered data interpolation problems have been developed (jointly with T. Foley).

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24. ADVANCED COMPUTER CONCEPTS $575,000 03
$100,000 Eqmt

George Michael, Garry Rodrigue, James McGraw

High Performance Systems

This category encompasses work in the second and third of the three DoE, Office of Basic Energy Sciences funded projects in mathematics and computer research at LLNL. All three projects contribute to the single goal of developing more effective high speed, large scale computers and methods for their use. The manner of working toward this goal involves close interaction with other DoE laboratories, universities, and computer manufacturers. LANL and LLNL sponsor several a series of special technical meetings to foster this collaboration.

The third of a planned series of meetings with these groups was held in mid-March, 1983. Known as the Oregon Meetings (OR83), the most recent one was entitled "The (Uncertain) Future of Environments and Workstations For Large Scale Computing." Attendance at the meetings is by invitation only. The purpose is to acquaint the groups with the anatomy of the large computational problems being worked on at DoE laboratories, principally LLNL and LANL.

The second Parallel Architectures Workshop (PAW83) was held in January 1983. This brings together DoE labs personnel and University researchers who are studying massively parallel computational structures. These meetings are smaller and more intense and from initial reports are very effective. Here also, manufacturers are invited to present their research for discussion by the attendees. The opportunity to exchange information with the most active researchers in the country has been valuable for everyone.

Last year we began yet another topical meeting series, this one on Monte Carlo Methods and Future Computer Architectures. The main reason for such a specialization is that Monte Carlo computations (also known, perhaps cynically, as the method of last resort) do not seem to map well onto vector or some parallel processors. We invited about forty scientists and Computists to discuss the use of Monte Carlo techniques. The meeting, held at Brookhaven National Laboratory in May, 1983, was very useful. For example, some powerful computational techniques were exchanged among the attendees; in the case of one program being used at one of the national laboratories, inclusion of this new methodology led to a factor of three computational speed up. Another report indicates that a new data structure being studied could make the general transport computation run faster on existing computers. More importantly, the new data structure can provide guidance for future computer designs. We expect to repeat this meeting every two years or so. A report and ealuation has just been completed and will be supplied to the

attendees.

The first of the two projects mentioned above studies languages that can exploit parallel architectures, the most likely form of super-speed computers in the near future. Collaborations with the University of Manchester (England), Colorado State University, and the Digital Equipment Corporation (DEC) have resulted in a significant upgrade of the data flow language SAL; the new language is called SISAL. Perhaps even more importantly, this collaboration has produced an intermediate graph form called, "IF1" that will greatly enhance the ability of all the collaborating sites to share the software products developed as a part of this research. For example, all the separate dataflow languages will be made to produce IF1-style graphs. So when the IF1 compiler is running on a given computer, a researcher can with minimal effort try any of the dataflow languages he wishes. Progress has also been made in the area of compilation techniques for SISAL and other applicative languages. In particular, cost/benefit analyses have been done for reference counting schemes (as a method to manage memory) and the use of non-strict arrays (as a means of enhancing concurrency). The implementation of an interpreter/compiler for SISAL was begun and will continue, as will research into compiler strategies for reducing memory requirements. We will continue research into execution strategies for handling the stream features in SISAL. We are continuing our efforts to extend SISAL with application-oriented features such as array processing.

The last project embodies a re-examination of the basic numerical techniques that serve to simulate large-scale physical processes. The goal of this effort is to generate a new set of numerical methods, compatible with each other, which are well-suited to future computer architectures and which embody the many advances of the last decade in the field of numerical analysis. The partial differential equations under study at LLNL are time-dependent and arise from hydrodynamics, electrodynamics, magnetohydrodynamics, transport theory and molecular dynamics. The development of a shock-capturing technique called the piecewise parabolic method for solving non-linear hyperbolic PDE's on irregular grids and for a multi-fluid medium has been completed. A two-dimensional local grid refinement technique for solving hyperbolic systems is being developed in which the local subgrids are dynamic. A basic proof-of-concept for the adaptive moving node method on one-dimensional transient problems was made as well as the development of a non-stiff and reliable node control algorithm. An algebraic interpretation of the multigrid method was made and the power of the method on highly stiff diffusion problems was demonstrated. A method for solving a two-dimensional advection-diffusion, singular perturbation problem was developed where the operator is split into a dominant and sub-dominant part cnsistent with the inherent directional property of the PDE.

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25. ADVANCED COMPUTING CONCEPTS ($0 in FY 1983) 03
Jack B. Dennis

Data Flow Computer Architecture

Our work is directed toward realizing practical high-performance computers embodying the data flow principle of instruction execution. The validity of the architectural principles of a data flow supercomputer has been established through the analysis and transformation of large Fortran benchmark programs for numerical weather prediction and numerical aerodynamics. Other applications will also be studied.

One area of concentrated effort is development of principles and algorithms for translating programs written in a high-level language (such as VAL) into machine-level program structures capable of full and balanced utilization of hundreds of data flow processing elements. This will provide the basic knowledge for building an optimizing compiler for data flow supercomputers. The second area of emphasis is the (custom) design of LSI part types for the main hardware units of data flow machines. This is needed to demonstrate that our performance predictions are based on realistic assumptions about hardware complexity and speed.

Other current work includes: extension and refinement of the programming language VAL; development of tools and methodology for the design of components of systems having packet communication architecture; and the application of coding and redundancy to achieve fault tolerance in data flow computer systems.

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26. ADVANCED COMPUTING CONCEPTS $99,807 03
Edward Fredkin, Tommaso Toffoli
Gerard Vichniac, Norman Margolus

Information-Preserving Models of Physics and Computation

This is a research project carried out by the Information Mechanics Group of the MIT Laboratory for Computer Sciences. During the last four years, this group has been active in investigating fundamental connections between physics and computer science, and encouraging exchanges between researchers in these fields. Information mechanics deals with dynamical systems that can be given two quite distinct interpretations. Depending on the viewpoint, these systems can be thought of as models of idealized physical processes or as physical models of computational processes. Such systems can be derived from conventional models of computation by adding certain constraints, so as to bring the computational model more into line with physics; alternatively, they can be derived from conventional models of physical processes by introducing certain assumptions that are required for finitary computational models.

The most basic assumptions that underly information mechanics are the following: (a) the structure and the laws of the dynamical system under consideration are such that their evolution can be computed exactly by finite means, and (b) the laws that govern the evolution of these systems are chosen so that the process is exactly reversible (which means that information is conserved).

This group has pioneered in showing that there are exactly reversible computational models that encompass all of the interesting behavior exhibited by real computers. This project will investigate reversible, discrete processes which share features of both physics and computation. Specifically, they are interested in (a) finite difference equations that are exactly reversible even when computed with round-off, (b) in the connections between symmetries and conservation laws in computational processes, (c) in seeing to what extent certain aspects of statistical physics and fluid dynamics can be interpreted purely in information processing terms, and (d) in the remarkable physical character of reversible cellular automata. The study of these topics may lead to a better understanding of the physical basis of computations, both in practical terms (e. g., efficient use of energy) and in theoretical terms (borrowing of physical concepts and mathematical methods). This study may provide new insights into computational models of physics and possibly into conceptual models as well.

This project is a new start in FY 1983.

DOE Applied Mathematical Sciences FY 1983

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27. ANALYTICAL AND NUMERICAL METHODS $95,000 01
Bernard J. Matkowsky

Research in Nonlinear Problems of Energy

This research continues theoretical investigations of bifurcation and nonlinear stability theories with emphasis on applications to combustion and flame propagation. Among the topics being examined the principal ones are: 1) formulation of cellular flame fronts; 2) effect of acceleration on the stability or propagating flames; 3) propagation of pulsating reaction fronts in solid fuel combustion; and 4) response of a system exhibiting bifurcation to small inhomogeneities.

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28. ANALYTICAL AND NUMERICAL METHODS $1,100,000 01
P. D. Lax
C. S. Peskin, M. H. Kalos, P. A. Whitlock,
J. Lebowitz, J. Percus, D. Heath, J. Marro,
M. L. Overton, J. Nocedal, J. Glimm,
O. McBryan, O. Betancourt, A. Harten,
O. Widlund, P. Bjorstad, E. Isaacson, M. J. Berger,
L. N. Trefethen, J. Goodman, R. LeVeque

NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

A topological argument has been used to show that no system of two conservation laws in two space variables and one time is genuinely nonlinear.

Work was started, with John Scheurmann, to apply the pseudo-cartesian method of Lapidus-Lax for calculating spherically and cylindrically symmetric flows, to calculate the reflection of an infinitely strong shock from the center of a sphere. An explicit solution for such a flow has been given by W. Noh.

A manuscript was prepared for the plenary session of the International Congress on problems solved and unsolved in linear and nonlinear partial differential equations

P. D. Lax

VORTEX METHODS FOR PROBLEMS WITH MOVING BOUNDARIES

This report covers two distinct but related projects. The first is concerned with flow past a flexible but inextensible leaflet; the second with flow past a rigid moving boundary such as a flat plate that is pivoted along a line. In both projects we consider two-dimensional flow at high Reynolds number.

In the leaflet project, we have a working computer program that has been tested on the following problem. The leaflet is placed in an unbounded fluid with the velocity at infinity prescribed. The upstream end of the leaflet is fixed. At the downstream end, a force is applied. The direction of the force is parallel to the free stream velocity. Initially, the leaflet is parallel to the free stream and an initial distribution of vorticity on the leaflet is specified. We find that the leaflet transiently develops a wave motion and the vortex sheet shed from the waving leaflet exhibits typical roll-up phenomena in the wake. The next step in this work is to apply the downstream force at a nonzero angle to the free stream velocity. In that case the leaflet models a sail with the fixed point as the mast.

In the pivoting-plate project, we use conformal mapping, and we solve the entire problem in the fixed, transformed domain. We have tested the method on the simple case in which the plate is fixed at zero angle of attack. The next test involves calculation of the torque when the plate is fixed at a nonzero angle of attack. We have prepared for this test by calculating the torque approximately using potential flow and free-streamline theory. Finally, we shall calculate the motion of the (massless) plate by solving at each time step for the motion that makes the torque zero.

The leaflet method can be applied to such problems as sails and parachutes and also to the study of natural heart valves. The pivoting-plate method can be applied to the study of pivoting-disc prosthetic heart valves.

C. S. Peskin

QUANTUM SYSTEMS

Our studies of quantum fluids have progressed along two fronts: (1) variational calculations of the ground-state properties of strongly-interacting quantum fluids, and (2) studies of scaling and finite-size effects inherent in the calculations themselves. In the first case, where more refined calculations take into account better wave functions, we have come to a deeper understanding of the equations of state of both normal (spin-saturated) and polarized (spin-aligned) phases of these low-temperature systems. In the second case, the study of the finite size effects in our many-fermion calculations has allowed us to indicate with greater accuracy the extent to which these simulations may be considered to be, both qualitatively and quantitatively, accurate representations of the corresponding bulk fluids.

An investigation into the ground state properties of two-dimensional He-4 has been initiated. Monte Carlo techniques for application to impurities in quantum fluids are being improved to allow the calculation of small differences, such as the exchange integral and the effective potential of a pair of He-3 atoms in He-4. Orientational order in quantum liquids and crystals is being studied to help elucidate the role of many-body interactions. Because of recent experiments on the momentum distribution of solid He-4, further work has been started on the corresponding theoretical prediction.

Another method for optimization of trial nodal surfaces is being developed for fermion systems. We are looking for the nodal surface that is the zero of the trial function which has maximum overlap with the GFMC solution. This method is currently being applied to model problems.

A novel possibility for the treatment of fermion systems has been devised. It consists in introducing a "mirror potential" to prevent the Green's Function Monte Carlo from converging to the boson ground state. Preliminary model calculations have given encouraging results.

M. H. Kalos et al.

QUANTUM CHEMISTRY

Within the limitation of the fixed node approximation, the Green's Function Monte Carlo (GFMC) method has been shown to be an excellent technique for the computation of atomic and molecular electronic correlation energy. In the case of the ten electron water molecule we have recovered 90 percent of the correlation energy with a simple one determinant molecular orbital trial wave function. The method is also capable of accurately computing excited electronic states. Results for the Be atom yield energies for the P-3 and P-1 first excited electronic states to within 0.1 eV of the experimental values.

For high Z atoms the Z/r coulomb singularity forces the GFMC algorithm to utilize small spherical domains due to the dense packing of the inner electrons in the vicinity of the nucleus. By adding and subtracting a Yukawa potential, the Hamiltonian may be rewritten as the sum of two terms, neither of which has the coulomb singularity present in the original form. In this way we may sample the potential directly, eliminating the spherical domains. A program to explore this technique has been written and is in the process of being debugged.

A new method has been devised to calculate the difference in energy between a molecular system and its constituent atoms. It is a perturbational estimate, well suited for Monte Carlo calculations, in which GFMC calculations for interacting and separated atoms are compared with variational calculations of the same systems. Preliminary calculations with model systems suggest that it is accurate enough for chemical systems since the perturbation expansion is in the energy difference rather than the total energies.

Our research offers the possibility of radically new methods in quantum chemistry and in turn of the theory of the kinetics of energy related chemical reactions. Another area which the accuracy and lack of basis set dependence of the GFMC method would be advantageous is in the study of electronic excited states.

P. A. Whitlock and D. Skinner

CHEMICAL KINETICS

This research deals with the computer simulation of the individual collisions of atoms and molecules that result in chemical reactions. One approach to this problem that will be used is to numerically solve the classical equations of motion for the reaction of interest. Emphasis will also be placed on Monte Carlo methods for the quantum equations of motion.

Testing of the four atom trajectory code to study the isotopic reactions of $(H+)_2 + H_2$ was completed and calculations initiated. Development on the assignment of states for the classical anharmonic triatomic oscillator continues.

The detailed understanding of macroscopic chemical reactions, for example, those in combustion systems, requires the elucidation of the reaction mechanisms at the microscopic level. Through these calculations predictions have been made both on systems accessible to experiment and on important intermediate reactions that as yet cannot be observed.

P. A. Whitlock

POLYMER SYSTEMS

We study the behavior of individual polymers and of systems of polymer molecules by considering simplified models of chain molecules. Our models view polymers as chains of connected units interacting via a Lennard-Jones potential. Thus, excluded volume effects are included. We expect that the properties of such systems will be characteristic of all polymers. We are particularly interested in the limit of very long chains.

We have employed a variety of algorithms in our simulations. We examined the structure and dynamics of dilute solutions containing a single chain in a solvent using the technique of molecular dynamics. In order to improve the computational efficiency for studies of multi-chain systems, we investigated a method called reptation, in which chain molecules move at random in a snakelike fashion. This provided an equilibrated state. Brownian dynamics algorithms were developed which enable us to follow the dynamical evolution of our multi-chain systems.

The influence of the attractive portion of the Lennard-Jones potential on the statics and dynamics of both single chain and multi-chain systems was investigated by reptation and molecular dynamics simulations. There was no significant effect at high temperatures; at low temperatures the attractions cause both the chains to be more compact and a slowing of the time correlation function.

The mean dimensions of multichain polymers were predicted to follow a scaling law involving the number of segments, the density, the dimension, and the critical exponent for the mean size of an isolated polymer chain. Simulations of both continuum and lattice systems in two and three dimensions were found to be consistent with the scaling relations.

Better theoretical understanding of conformational and dynamic effects in polymers is needed in their use as structural materials and in studies of biological macromolecules.

M. H. Kalos and J. Lebowitz

CLASSICAL FLUID SYSTEMS

We are concerned with the study of interface effects on the structure and dynamics of simple fluids. The ultimate aim of the research is to suggest the structure of theories which will account for the flow of liquids in the presence of inhomogeneities, such as interfaces with gases or material boundaries. One can thereby formulate suitable

macroscopic models and boundary conditions for inhomogeneous flow. The hope is to be able to go beyond merely analyzing known flow behavior to the point where, for example, pipes with reduced friction against flow can be invented.

The technical work involves Monte Carlo (for static properties) and molecular dynamics (for dynamical properties). We are testing new Monte Carlo methods intended to give selectively better statistics for properties of interest near the inhomogeneous regions. Of particular interest is the transverse structure factor near a hard wall bounding an argon-like fluid.

An alternative technique was developed for measuring the local density along a line normal to the average vapor-density interface. We are now analyzing the structure of the transverse correlations in fourier space.

The applications of this work are ultimately twofold. First, the calculations will enhance our understanding of nucleation processes in vapor-liquid systems. Second, the research attempts to elucidate the microscopic processes that underlie boundary effects in inhomogeneous fluid flow.

M.H. Kalos, J. Percus, and D. Heath

ALLOY SYSTEMS

This research deals primarily with the properties of matter that is not in thermodynamic equilibrium. In solid systems we are principally concerned with the development of grains in alloys quenched from the melt. This is of great importance since the metallurgical properties are determined in large part by the imperfections that develop.

Our primary tool in these investigations is computer simulation of atomic models with some form of dynamics that drives the system toward equilibrium. Of necessity, the thermodynamics of these systems must be investigated when they are not adequately known. For alloy systems, we use Kawasaki kinetics in which adjacent atoms are exchanged when such a change is energetically favorable. For fluid systems, specific atomic force laws are used along with molecular dynamics as an algorithm.

The program for the simulation of binary alloys was modified to include the effect of an external electric field, and the revised program was put into production on a CMCL PUMA. Calculations were run at sufficient temperatures and concentrations to map out the parameter space. These results are now being analyzed.

During the last year some systematic attention has been given to optimal sampling methods along the lines of the algorithm of Metropolis, Rosenbluth, Rosenbluth, Teller and Teller. Specifically, the idea is to incorporate knowledge of exact or approximate collective modes in the generation of trial moves. Specific proposals have been made for Ising systems which include ideas of renormalization group for classical systems. The question of optimal sampling schemes is interesting also in

the context of computer architecture since the conclusion may be drawn that although the Metropolis method for lattices superficially involves only lattice connections. The optimal sampling will require more general communications patterns.

M.H. Kalos, J. Lebowitz, and J. Marro

NUMERICAL OPTIMIZATION

Large scale sum of norms optimization applied to problems from collapse load analysis - The particular collapse load problem of interest requires minimizing an integral of the absolute value of a gradient of a function in 2D, subject to some constraints. Strang has shown that the solution is a characteristic function with jump discontinuities. Our algorithm is designed to minimize a discretized version of this problem. Thus we hope it to be useful, ultimately, to solve related problems for which analytic solutions are not known.

An algorithm for these special non-smooth optimization problems has been implemented, although some details remain to be decided. The initial numerical results are quite encouraging. Of particular concern has been the matter of dealing with the inherent degeneracy in the problem. A solution based on a suggestion of A. Dax is being considered and tested.

This problem arises in the design of structures, where the concern is to ensure that the structure is strong enough not to collapse under a given load.

M. L. Overton

INVERSE EIGENVALUE PROBLEMS

The inverse eigenvalue problem consists in choosing some parameter values so that a particular matrix function of these parameters has prescribed eigenvalues. There is a large literature on this subject, particularly concerning existence and uniqueness results. We are concentrating on numerical methods for problems where it is assumed that a solution exists.

A Newton-type algorithm has been implemented. We are particularly interested in cases where the solution matrix has multiple eigenvalues. We have been able to demonstrate numerically and prove theoretically that the algorithm does have quadratic convergence even in the presence of multiple eigenvalues. Several interesting variations of the inverse eigenvalue problem are being considered - for example, a problem arising in factor analysis.

This problem also arises in structural analysis. In this case the goal is to ensure that the natural frequencies of the structure are as prescribed, in a range outside any potentially dangerous values, e.g., the frequencies associated with wind, earthquakes, or waves. It also arises in a number of other applications including quantum physics and

spectroscopy.

M.L. Overton and J. Nocedal

PROJECTED HESSIAN UPDATING ALGORITHMS FOR NONLINEARLY CONSTRAINED OPTIMIZATION

The constrained optimization problem requires minimizing a function subject to nonlinear constraints on the variables. Quasi-Newton methods are used to solve these problems when the Hessian matrices of the function and constraints are unavailable or too expensive to use. The standard approach is to approximate a full Hessian of the Lagrangian function, an nxn matrix, where n is the number of constraints. We are interested in approximating some form of projected Hessian, i.e., a matrix projected into the null space of the relevant constraints. This type of approach has a number of advantages.

We have been considering quasi-Newton algorithms for solving nonlinearly constrained optimization which approximate a projected Hessian, rather than a full Hessian of a Lagrangian function. A Broyden method which approximates a rectangular matrix is also being considered. We have made some numerical experiments which suggest that these algorithms may be very useful. We have also proved some two-step superlinear convergence results.

M. L. Overton and J. Nocedal

COMPUTATIONAL AND STATISTICAL METHODS FOR FLUID INTERFACES

Fluid interfaces arise as material boundaries, slip lines, and shock waves. Methods based on front tracking have been developed to study these interfaces numerically. The numerical methods have been validated by a test against known analytic, numerical, and experimental solutions in a variety of problems drawn from oil reservoir simulation, inertial confinement for controlled nuclear fusion, and shock tube experiments.

In studies of oil reservoir simulation, fingering instabilities of an oil-water interface were studied both deterministically and statistically. It was shown that geometrical effects (convergence vs. divergence of the flow field) can have a very strong influence and can stabilize (for diverging flow) or destabilize (for converging flow) an interface which on other grounds had the opposite character. The stabilization is a phenomenon of saturation or limitation on the disturbance amplitude and thus does not show up in a linearized stability analysis.

Studies of the Rayleigh-Taylor instability show that pinchoff and droplet formation should occur in a two dimensional model, leading to filaments which are vortex sheets or slip lines after pinchoff has occurred. This is a mechanism for transport of vorticity from the interface into the fluid interior which is totally distinct from the usually discussed mechanism of viscous diffusion.

The shock tube calculations show high quality resolution of the flow field on coarse grids.

The applications cited are governed by hyperbolic and/or elliptic equations. In the context of hyperbolic equations, front tracking is a moving grid of one dimension lower than the interior, which follows or moves with the tracked wave. The motion of the tracked wave is governed by Rankine-Hugonoit relations and the solution of Riemann problems, or for several waves meeting in a point, by shock polars. The solution of Riemann problems in the large, in higher dimensions and with nonlocal data poses a series of mathematical problems of a fundamental nature. Progress was made on this program. The data structures and coupling between interior and tracked waves have been upgraded in recent work.

In the context of elliptic equations, interfaces give rise to coefficient discontinuities and singular source terms. The correct computation requires an adaptive grid and an efficient solution algorithm. The grid construction was improved to be more robust near a region of pinch-off. The solution algorithm was speeded up by several methods, including the use of multigrids, combined necessarily with the adaptive grids. Also network software was developed to allow a uniform user interface for the CRAY or FPS used as an attached processor on a host machine.

Fluid interfaces arise in many methods for production of energy and an ability to calculate accurately with them is of relevance to DOE activities.

J. Glimm, O. McBryan, et al.

EQUILIBRIUM, STABILITY, AND TRANSPORT FOR STELLARATORS

The three-dimensional equilibrium and stability code BETA has been used to calculate the Mercier criterion for local stability and for neoclassical transport based on Boozer's theory. The code permits effective representations of the magnetic field in terms of Clebsch flux functions and potentials. Formal Fourier series in flux coordinates yield reliable estimates of the parallel current and of drift surfaces. Applications have been made to the ATF-1 experiment under construction at ORNL. It has been shown that a satisfactory beta limit can be achieved by introducing a vertical field to shift the magnetic axis outward. Other cases studied were the newly proposed experiment at Garching, the W VII-AS Stellarator, and the existing W VII-A and Heliotron E Stellarators.

O. Betancourt

ACCURATE AND STABLE SCHEMES FOR SHOCKS

During the past two years, we have constructed various classes of explicit and implicit difference schemes for computing solutions with shocks of hyperbolic conservation laws in one space variable. The schemes are (a) total variation diminishing, and (b) second order accurate. These schemes combine robustness with high resolution. It is well known that for linear equations no linear scheme has both property (a) and (b).

During this year the method was implemented for various problems. The implicit scheme has been used to calculate efficiently steady states as limits of time dependent ones.

The methods work well for two dimensional problems by breaking them down to one dimensional fractional steps.

A. Harten

SOLVING ELLIPTIC FINITE ELEMENT PROBLEMS ON REGIONS PARTITIONED INTO SUBSTRUCTURES

Special iterative methods have been developed for the solution of elliptic finite element problems on regions regarded as unions of subregions. If the elliptic problem restricted to the subregions can be solved by a direct method, the whole problem is reduced to finding the values of the variables associated with the nodes on the curves or surfaces which partition the region. Several preconditioned conjugate gradient methods have been introduced. Numerical experiments and theoretical results show that some of these methods can be very efficient. A comparison has also been made with similar methods developed by Golub and Glowinski and their co-workers.

O. Widlund and P. Bjorstad

NUMERICAL METHODS FOR QUEUING NETWORKS

Work has begun on developing fast methods for the numerical solution of the Kolmogorov balance equations which provide the stationary probability distribution for queuing networks. In simple cases, methods of decomposition of separation of variables can be applied to give easy answers. In recent papers, Linda Kaufman of Bell Laboratories, has considered more general problems of this kind and made considerable progress exploiting decomposable subsystems, etc. We have designed new algorithms which have been shown to be optimal for at least one interesting family of problems. We have made preliminary experiments with two queue systems which are quite promising. In contrast with sparse matrix techniques, our methods show promise of becoming equally useful for three and more queues.

O. Widlund

NUMERICAL CONFORMED MAPPINGS

Work has continued on providing a complete theory for an interesting method developed by Fornberg. In addition, Tom DeLillo has done extensive work on combining Fornberg's and similar methods with more elementary ways in order to increase the efficiency of the methods and to handle almost intractable cases.

O. Widlund

UPGRADING OF CAPACITANCE MATRIX CODES

In our existing, commonly available codes for the solution of Helmholtz's equation on general regions in two and three dimensions, the capacitance matrix equations were solved by a least squares approach and the standard conjugate gradient method. We now have extensive experience with solving these systems with conjugate gradient-like methods designed to handle nonsymmetric problems. These iterative methods have been extensively studied in recent years in particular at the computer science department at Yale.

O. Widlund

CLIMATOLOGY AND METEOROLOGY

Deciding if increases in carbon dioxide, dust, and other pollutants in the atmosphere will produce an irreversible change in the climate, i.e., greenhouse effect, is an important problem. In this connection, we have been developing a fully implicit difference scheme that is accurate for long term calculation of global atmospheric models. With such mathematical systems, we can analyze how, when, and where ice ages or desert ages might develop. Work is being done in collaboration with S. E. Cohn, M. Ghil, and D. Marchesin.

We are developing accurate ways to incorporate observations made by space satellites into the standard numerical weather prediction procedures. This work is being done in collaboration with S. E. Cohn, D. Dee, and M. Ghil.

E. Isaacson

GRID REFINEMENT AND MESH GENERATION

The main area of research this year was in adaptive methods for the numerical solution of pde's, in particular, for steady state transonic flow in two dimensions. It is now widely accepted that realistic transonic flow calculations require some type of multiple mesh or grid refinement strategy. Grid refinement is necessary because it is impractical to use globally fine meshes that adequately resolve flow at the leading and trailing edges and at shocks. Multiple meshes are useful to ease the grid generation problem around complex configurations. Furthermore, the mesh generation should be automatic. It is not always possible to determine in advance of a computation where the regions needing refinement are (for example, the shock location), and how fine to make the grid spacing there. Thus some type of adaptive refinement strategy is needed.

In one such adaptive mesh refinement algorithm the grid refinement is accomplished by generating locally uniform fine grid patches which are superimposed on an underlying global coarse grid. If several such grid patches are needed to attain a given accuracy in the solution, they are recursively nested. Algorithms have been developed which automatically estimate the local truncation error in the solution on a given grid. This is used as the criterion for refining the grid. We also have algorithms to automatically generate the locally uniform fine grid patches

to include the regions of high error. In addition, a simple data structure to keep track of the multiple grids has been devised.

In more recent work, this adaptive mesh refinement algorithm has been extended to solving the Euler equations in two dimensions for steady flow about an airfoil. By refining the grid at the leading and trailing edges of the airfoil, we have been able to recover the accuracy of the solution on a grid which is uniformly refined over the entire flow field. Furthermore, because of the simple user interface which results from using the locally rectangular grid patches, we have been able to use an existing Runge-Kutta finite volume method (FL052) to integrate the equations in the interior of each grid. Special procedures are needed at the interface between a coarse and a fine grid. We have developed special difference equations which maintain the conservation form of the integrator, and thus guarantee the correct shock location. This is important since a fine grid patch will sometimes be needed at a discontinuity, and so there will be a grid interface near the shock. More general types of conservative interface conditions, e.g., for grids which are rotated with respect to each other, or grids which do not meet at a coordinate line, are being developed.

The final project studied this year was the stability properties of interfaces where the mesh on one side of the interface is refined in both time and space. We have been able to prove stability for explicit, three point, dissipative finite difference schemes which use two time levels. For schemes with more than two time levels, the stability question reduces to checking a simple, scalar equation for values of a parameter on the unit circle. In addition, stability can be proved for the nondissipative case of the Leapfrog scheme if the meshes overlap, so that some interpolation is needed at the interface.

M. J. Berger

STABILITY THEORY

In stability theory for finite difference methods, we extended previous work which developed a connection between the dispersive propagation of parasitic numerical waves and the instability of numerical boundary conditions. This provides a physical interpretation of the well known stability theory of Gustafsson, Kreiss, and Sundstrom. During the past year we first made these results rigorous. We then worked on extensions of these ideas to numerical models containing two boundaries rather than one, as is usual in practice. Here repeated reflection of waves between the boundaries can generate new forms of instability. On the other hand by forcing small reflection coefficients one can guarantee stability.

A more theoretical improvement on a stability result, known as the Kreiss matrix theorem, establishes a connection between the stability of families of difference operators and the behavior of the associated resolvent matrices.

L. N. Trefethen

NUMERICAL CONFORMAL MAPPING

Our work in numerical conformal mapping concerns the numerical implementation of the Schwarz-Christoffel transformation, which maps a standard region in the complex plane conformally onto a polygon. Despite the long history of the Schwarz-Christoffel idea, it is only through our recent work that it has become a practical tool for general polygonal domains, because of the difficult associated numerical problems of finding certain unknown "accessory parameters" and of integrating the S-C integral accurately.

We developed a portable version of the Schwarz-Christoffel computer package "SCPACK", which has been distributed to several users. We studied applications and extensions to several areas, including: grid generation; free-streamline problems for fluid flow in the presence of jets, wakes, or cavities (via the hodograph transformation); computation of electrical resistances; solution of Laplace's equation subject to oblique derivative boundary conditions, as occurs in queuing theory and in modeling the Hall effect for semiconductors. This work is of mathematical as well as of practical interest, because the various Schwarz-Christoffel problems differ in challenging ways: the polygon may contain unknown geometrical parameters to be determined implicitly; it may be a Riemann surface with branch points; it may be a periodic surface requiring a modified form of the Schwarz-Christoffel integrand.

L. N. Trefethen

ACCURATE AND STABLE SCHEMES FOR SHOCKS

Numerical computations involving shock waves have suffered from an unhappy tradeoff between accuracy and stability. Accurate schemes produced spurious numerical oscillations near shocks, while stable schemes were too inaccurate for practical two or three dimensional computations. Recently A. Harten has constructed schemes that are second order accurate while retaining the strong nonlinear stability property of being total variation diminishing (TVD). Since Harten's schemes were one dimensional it was natural to try to extend his results to two and three dimensions. Instead, we found that such schemes do not exist; a TVD scheme in more than one dimension is at best first order accurate. However, two dimensional computations based on schemes like Harten's work quite well, so theoreticians must find another stability definition, weaker than TVD, that still guarantees convergence.

In one dimension the commonly used MUSCL scheme of Van Leer, properly implemented, is TVD. Many schemes have the property that rarefaction waves are spread insufficiently or not at all by the difference scheme. We have analyzed this phenomenon and shown that it can be cured by adding a small amount of extra smoothing.

J. Goodman and R. LeVeque

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29. ADVANCED COMPUTER CONCEPTS $600,000 03
M. H. Kalos, J. T. Schwartz, R. Bianchini
VERY HIGH PERFORMANCE PARALLEL COMPUTERS

The rapid development of VLSI technology is making it feasible to construct highly parallel computing assemblages involving thousands or tens of thousands of tightly linked computing elements, all cooperating for the rapid solution of single tasks. Machines of this class could attain instruction rates of tens or hundreds of billions of instructions per second. To make such machines effective, appropriate hardware and software design choices are required. A key hardware issue is the design of an interconnection network capable of moving data at very large rates between processors and memory. This network must also support very high speed interprocessor synchronization problems. Key software issues are the definition of data structures and operating systems which allow the concurrent operation of very large numbers of cooperating processors, and of programming language features which make it possible for existing code libraries to be adapted for massively parallel execution.

During the last year a two-processor Ultracomputer prototype was constructed and a first operating system installed. The latter is a "master-slave" adaptation of the UNIX (TM-Western Electric) system. We used the DARPA MOSIS line to fabricate successfully a simplified initial version of the VLSI systolic queue on which the nodes of the Ultracomputer network is based. A faster version has been prepared for fabrication.

Our simulation work has continued for both applications and hardware. Network and cache simulators are now operational and have produced significant data for hardware cache design and important confirmation of the need for combining requests in the network. LLNL's SIMPLE code has been ported for our instruction level multiprocessor simulator and its efficiency on an Ultracomputer is being studied.

Finally, we have new results on the theory of automatic verification of parallel programs, on the design and analysis of parallel algorithms, and on abstract models of parallel computation.

Next year, we expect that an eight-processor prototype using the newly designed processor board will be functional using a bus for access to PUMA memory. A cache which is currently being designed should also be functional during the next year. In addition, substantial progress should be made towards a switch network using VLSI technology based on the current VLSI design effort.

DOE Applied Mathematical Sciences FY 1983

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30.	SPECIAL PROJECTS/	$100,000	04
	RESEARCH COMPUTING FACILITY	$260,000	Eqmt
	M. Goldstein, E. Franceschini		

The Research Computing Facility (RCF) provides the computational resources needed to support the ongoing basic research in applied mathematical sciences. It serves as a testbed for the evaluation and development of new computing capabilities. Maintenance and development of the RCF, including integration and evaluation of emerging computing technologies, are a focal point for collaborative interaction with other DOE research sites and with researchers in computer science throughout the University and industrial community.

The experimental effort places special emphasis on issues relating to distributed computing environments and the applicability of varied computational resources to DOE scientific researchers. The goals of the experimentation are to: (a) provide a variety of computer facilities to the CMCL community, (b) acquire and devise means to easily enable communications among the various hardware and software elements composing the Research Computing Facility, and (c) discover and implement means that reduce the impact on the user of the complexity inherent in multicomputer environments.

The new ARPANET protocols, TCP and IP, have been installed in conjunction with the mandated network-wide upgrade. The ELF system for ETHERNET access has been retired. We are now using the UNIX-based implementation developed by the University of California at Berkeley and BBN, Inc., under DARPA sponsorship.

A Floating Point Systems Array Processor has been acquired and installed as a satellite to a VAX-11/780 on our local network. ARPANET access is available.

ETHERNET has been chosen for a pilot coax-based Courant Institute network implementation. A VMS and UNIX VAX have been connected and are successfully running the DARPA TCP/IP protocols. The local network now contains ten VAX's and five PDP-11's. These will be connected to the ETHERNET.

DOE Applied Mathematical Sciences FY 1983

OAK RIDGE NATIONAL LABORATORY
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31. ANALYTICAL AND NUMERICAL METHODS $360,000 01
R. C. Ward, M. T. Heath, D. G. Wilson,
A. D. Solomon, L. J. Gray, R. E. Funderlic

Applied Analysis

Research in Applied Analysis is carried out in three areas, namely moving boundary problems, material science, and stochastic analysis. Researchers working in these areas develop mathematical and computational models of physical structures and processes. Work in moving boundary problems concerns heat and mass transfer with accompanying change of phase. For the last two years attention has been focused on modeling binary alloy solidification. A steady stream of reports and journal articles has documented our progress in producing more and more comprehensive, sophisticated and useful models of this process. Insights gained from these results will be used to develop models for similar but more complicated problems. Research in material science is directed toward fracture mechanics with emphasis on the mathematical consequences of the newly discovered dislocation-free zone at the crack tip. Our research in this area is concluded this fiscal year. Research in stochastic analysis concerns the modeling of disordered systems such as amorphous solids and liquids. This work has also become involved with alloy solidification but nonequilibrium or "ultrafast" solidification resulting in amorphous alloys.

Computational Mathematics

The focus of this work is on problems involving sparse matrices in the areas of systems of linear equations, eigenvalue problems, and least squares approximations. Recent emphasis has been placed on development of algorithms suitable for parallel computers and other advanced computer architectures. Our algorithms for sparse least squares problems have been extended to include very general constraints and updating, with no restrictive assumptions regarding rank. Another offshoot of this work is the development of an elimination-based direct method for square linear systems that is suitable for parallel computation. Our work on the force method for structural analysis has lead to algorithms for computing sparse null space bases. We have developed new algorithms for computing small singular values of large sparse matrices and for computing the singular value decomposition of a product of two matrices without forming the product explicitly. Our work on the M-matrices arising from queuing networks and Markov chains has continued, including the development of a combined direct/iterative method for solving linear systems involving such matrices.

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32. INFORMATION ANALYSIS TECHNIQUES $325,000 02
R. C. Ward, T. J. Mitchell, M. D. Morris,
J. J. Beauchamp, K. O. Bowman, T. Wright

Statistical Methods

The Statistical Methods research effort is divided between two research projects, Computational Statistics and the Analysis of Large Data Sets. Research in the Computational Statistics Project has emphasized the following areas: computer-aided experimental design; computer-oriented statistical inference related to the computation of distributional properties of estimators for widely-used probability models; and computational algorithms for performing linear dependency analysis on ill-conditioned data matrices using modern numerical linear algebra techniques. Research in the Analysis of Large Data Sets Project has focused on the following topics: evaluation of widely-used classification procedures common in large data sets with mixed data types; estimation in the area of data-based transformations; and evaluation of methods to analyze data arising from imperfect sampling frames. A draft of the planning document, "Program Directions for Research in Statistical Methods," has been completed in collaboration with members of the statistical community and other statisticians within the Applied Mathematical Sciences Program.

DOE Applied Mathematical Sciences FY 1983

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33.	SPECIAL PROJECTS/	$65,000	04
	RESEARCH COMPUTING FACILITY	$75,000	Eqmt
	R. C. Ward, D. G. Wilson		

Late in fiscal year 1983 the Mathematics and Statistics Research organization acquired a Digital Equipment Corporation VAX 11/780 superminicomputer and a "starter set" of peripheral equipment. This machine will serve as the principal item of our Research Computing Facility (RCF). Acquisition of additional equipment necessary to make the RCF fully operational has begun. Connection to the Defense Data Network (MILNET/ARPANET) is expected early in 1984. The RCF will be used to explore innovative approaches to scientific computing, including the simulation of advanced computer architectures, and to communicate with researchers at other Department of Energy facilities.

DOE Applied Mathematical Sciences FY 1983

BATTELLE PACIFIC NORTHWEST LABORATORIES
Statistics Section, Energy Systems Department
Computers & Info. Systems, Engineering Physics Dept.
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34. INFORMATION ANALYSIS TECHNIQUES $500,000 02
D.L. Hall, W.L. Nicholson, R.J. Littlefield, D.B. Carr, P.J. Cowley, R.A. Burnett, J.J. Thomas, M.D. Erickson

Analysis of Large Data Sets and Statistical Methods

The goal of Applied Mathematical Science research at PNL is to develop new methodologies for the analysis of large data sets. To effectively utilize the ever growing quantities of increasingly complex energy-related data requires new techniques in data analysis, visual display and data management. This integrated statistics and computer science research project is supported by the Research Computing Facility, a statistical laboratory dedicated to large data sets that serves as a test bed for new statistical methods and innovative approaches to analysis. A review panel of expert statisticians and computer scientists from government, universities and private industry meets periodically to evaluate and guide the research.

Statistical research focuses on exploratory data analysis for large data sets and emphasizes highly interactive graphical analysis techniques. Specific topics addressed are new techniques for expanding the number of dimensions that can be displayed and manipulated, the definition and automatic detection of "interesting" structure in data sets and a theory of graphical inference.

Analysis of Large Data Sets - Data Management and Display Systems

With most current data management systems and techniques, the difficulties of large data set analysis are compounded by the inadequacy of facilities to assist the analyst in managing, controlling and maintaining descriptions of multiple data sets, subsets and analysis results, all of which tend to proliferate during exploratory analysis. This proliferation of data and derived results can be viewed as an evolving sequence of "data analysis environments." Data management research focuses on the definition, manipulation and control of these data analysis environments. Specific areas of research include data modification descriptions, data dictionaries/directories, and interactive control and graphical representations of data analysis environments.

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Department of Statistics
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35. INFORMATION ANALYSIS TECHNIQUES $257,000 02
John Tukey

Interactive Graphical Data Analysis

We are developing improved techniques for interactively analyzing numerical data. A major task is the refinement of current data analysis software and the development of new algorithms. The emphasis is on the effective use of graphical outputs to communicate results to the data analyst. This will require exploration of graphical techniques for presenting the results of otherwise conventional analyses, and also the development of new analysis techniques for which the results are essentially graphical.

We will also define a computer configuration that takes advantage of new mid-sized machines to provide powerful support for interactive data analysis. This will be acquired during the second year and will be our primary equipment for software development.

Progress was made on new types of robust estimates of location called "compromise" estimates. Two types of estimates were studied: a [illegible] kind of M-estimate called a psi-compromised M-estimate, and a gap-compromised estimate which has as its underlying foundation the same working mechanism which has made many M-estimates so successful, namely, the downweighting of observations that are extreme with respect to the rest of the data. The estimates discussed here are constructed to do well when the data are from one or two distributions.

The procedures developed can be generalized easily for optimization over any finite set of distributions. An obvious compromise of this sort would be one among the distributions Gaussian, slash, and one-wild that compose Tukey's three corners.

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36. ANALYTICAL AND NUMERICAL METHODS $60,376 01
John R. Rice

Numerical Solution of Elliptic Partial Differential Equations

ELLPACK is a cooperative project led by John Rice at Purdue University for the study and development of software and methods for solving elliptic problems. Cooperating institutions include the University of Texas, Yale, Harvard, the National Bureau of Standards, South Carolina, Southern California, Exxon Research and Bell Labs. The project includes the ELLPACK system which has about 40 software modules for all or some of the steps in solving an elliptic problem. One can naturally state an elliptic PDE and request that it be solved by one (or more) of the modules. The objectives of this system are (a) to support extensive performance evaluations of numerical methods, (b) to solve elliptic problems of moderate size, (c) to develop prototypes of large scale software systems for elliptic problems, and (d) education. In the 1981 FY a new version of the ELLPACK system will become operational which will be standardized, thoroughly documented, and portable. New software modules that will be added include general piecewise polynomial collocation, higher order difference methods, blending function methods and multigrid methods. Systematic performance evaluations will be made for (a) methods for 3D problems on rectangular domains, (b) the effect of derivatives in the boundary conditions on various methods' performance, (c) methods for 2D problems with general domains. Research will continue on the development and analysis of new methods that may eventually be included in the ELLPACK system.

WILLIAM MARSH RICE UNIVERSITY
Department of Mathematical Sciences
Houston, Texas 77001

37. ANALYTICAL AND NUMERICAL METHODS $93,139 01
Richard A. Tapia, John E. Dennis

Extension of Quasi-Newton Methods to Constrained Optimization and to General Systems of Nonlinear Equations and Inequalities

This research is a continuation of work to extend quasi-Newton methods for unconstrained to constrained optimization problems and to construct effective quasi-Newton methods for large scale problems. Considerable time will be spent on global strategies for constrained optimization. The work summarized here is not based on altering existing quasi-Newton methods to make them applicable to important problems in numerical optimization. Rather, it follows the more ambitious approach of identifying the principles behind the successful methods and then applying those principles to tailor new algorithms for specific classes of problems. Although the long term research goals of the investigators are primarily concerned with the nonlinear programming problem, much of this work is concerned with methods which are new even in the unconstrained case. An objective is to develop computationally effective methods and a primary target is to reduce the cost of the linear algebra involved in each iteration even at the expense of some increase in the number of iterations that would be necessary to solve the problem by more traditional quasi-Newton methods. Thus this class of methods could be useful only in those cases when forming certain coefficient matrices and solving the resulting linear systems is a significant part of the cost of an iteration. Even in such cases enough algebraic work must be saved at each step to make up for any increase in the number of iterations and in associated calls to user supplied function subroutines. The work is progressing.

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38. ANALYTICAL AND NUMERICAL METHODS $65,000 01
R. J. Gelinas

Moving Finite Elements in 2-D

This research investigates the mathematical and computational properties of the moving finite element (MFE) method in both existing and advanced computer environments. The capacity of the MFE method to solve numerically large classes of transient, nonlinear PDE problems which may involve multiple, large gradients in 2-D is of primary interest, and some supportive analysis is also carried out in 1-D. Recent results in this effort have demonstrated that the MFE method may be particularly well-suited to resolving problems in numerous DOE program areas which involve non-equilibrium hydrodynamics and transport effects and which would include shocks in gases, liquids, and solids; such detailed combustion processes as ignition, quenching, and deflagration-to-detonation transitions; thermal hydraulics; lubrication; continuum mechanics; flow in porous media; free-electron and chemical laser processes; and numerous areas of plasma physics in both weapons and civilian energy systems.

The present MFE research in 2-D focuses upon such general technical topics as optimality of various node movement criteria and properties in moving finite element methods, as well as their logical analogues in finite difference methods; the study of topological properties of PDE node movement methods, as contrasted to data structure requirements of PDE mesh refinement methods; alternative MFE basis functions; vectorization properties of the MFE method; ande potential applicability of the MFE method in advanced computer environments. Specific topics in this year's MFE research include the development of node controlling regularization functions in 2-D grid meshes; efficient methods of solving the large systems of linearized equations for the nonlinear ODE's of the MFE method in 2-D; and the study of alternative MFE grid meshes which would be effective for use with dynamic ADI methods and for resolving complex fluid structures in multidimensional shocks.

This research is being performed in close collaboration with Professor Keith Miller and graduate students in the Mathematics Department at the University of California, Berkeley.

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39. ANALYTICAL AND NUMERICAL METHODS $200,000 01
L. F. Shampine, D. E. Amos

Mathematical Software

Fundamental research into the numerical solution of ordinary differential equations will lead to an improved understanding of the task and to more efficient and reliable software: New understanding and improved estimates of local errors will be achieved. Several kinds of standard methods will be made more efficient and reliable. Global (true) error estimates will be devised. New methods for the solution of stiff problems will be proposed.

A comprehensive package of Bessel functions of complex argument and non-negative orders will be constructed. For maximum applicability and efficiency, each code requires the use of several methods. This necessitates fundamental mathematical and software research as well as extremely careful development and testing.

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40. ANALYTICAL AND NUMERICAL METHODS $400,000 01
Robert J. Kee, S. B. Margolis, L. R. Petzold,
J. F. Grcar, M. D. Smooke

We are concerned with the solution of disparate-scale partial differential equations (pde); our approach is both analytical and computational. Although the results of our work are applied generally, one unifying theme is our interest in the problems that arise in combustion modeling. On the analytical side we are developing asymptotic models that explain instabilities in flames. A particularly interesting recent result is the prediction of cascades of bifurcating solutions as premixed flames become increasingly unstable. On the computational side, we concentrate on large systems of stiff pdes, such as those that occur in models involving systems of complex chemical reactions. We are working implicit methods, such as backwards differentiation formulas and implicit Runge-Kutta, that deal effectively with the widely varying time scales that are present in chemical kinetics models. In addition, we are developing adaptive gridding methods that are required to resolve accurately localized behavior such as flame fronts. The final aspect of our program is the development of stable iterative methods to solve the systems of nonlinear equations that arise in implicit algorithms.

DOE Applied Mathematical Sciences FY 1983

STANFORD UNIVERSITY
Systems Optimization Laboratory
Department of Operations Research
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41. ANALYTICAL AND NUMERICAL METHODS $280,500 01
George B. Dantzig, Richard W. Cottle
Walter Murray

Systems Optimization Project

The Systems Optimization Project is one of the principal activities of the Systems Optimization Laboratory (SOL), Department of Operations Research, Stanford University. The work of the project is directed toward the development of effective numerical methods for practical optimization and equilibrium problems arising in the energy field and other areas. Behind this overall objective, research at SOL includes a range of different aspects: definition and characterization of useful problem categories; creation and design of algorithms; thorough study of the mathematical and numerical properties of algorithms; implementation with sound numerical and programming techniques; and evaluation and comparison of algorithms. Currently research is proceeding in the following areas: methods for staircase linear programs; analysis of conjugate gradient and sparse quasi-Newton techniques for unconstrained optimization; extensions to the MINOS/AUGMENTED code for large scale constrained optimization; development of several projected Lagrangian methods for nonlinearly constrained optimization problems; development of truncated Newton methods; extension of quadratic programming subproblem methods to solve large problems; and methods for sparse linear least-squares.

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42. ANALYTICAL AND NUMERICAL METHODS (No Fund Extension) 01
Gene H. Golub

Numerical Analysis

The purpose of this research is to devise numerical methods for solving problems arising in applied mathematics and data analysis. The main focus of the research is on matrix computations. There are several areas which are being considered. The first is that of solving large systems of linear algebraic equations which are sparse. These systems frequently arise from partial differential equations and as such, the matrices have special properties. In addition, one can frequently take advantage of the fact that the matrix operator can be split into two or more parts, one of which is "easy" to solve. We are currently emphasizing problems where the matrix of coefficients is not symmetric but the system is positive definite. This set of problems seems to be of more significance than originally assumed. In addition, we are considering large sparse least squares problems and for these problems we are also developing iterative procedures in combination with splitting methods.

In the usual data fitting problem, it is assumed that the model is known precisely. We have considered problems where some of the data is known exactly but not all of the variables are not known precisely. When the problem is linear, this leads to a matrix computation involving the singular value decomposition. We are currently developing software for solving these important practical problems.

Inverse eigenvalue problems play an important role in many fields, including geophysics. We are devising algorithms for solving specialized classes of problems. These algorithms represent a substantial improvement in numerical accuracy and computer time over the previously known algorithms.

UNIVERSITY OF CALIFORNIA, BERKELEY
Center for Pure and Applied Mathematics
Berkeley, California 94720

43. ANALYTICAL AND NUMERICAL METHODS $275,000 03
R. J. Fateman, W. Kahan

Research in the Design and Implementation of a Comprehensive Facility for Scientific Computation

The goal of this work is to incorporate the extensive experience of the investigators into a unique scientific software facility representing the uncompromisingly best capabilities which can be made available in the new breed of large address space, low cost, high performance computers (typified in current product lines by the Digital Equipment Corporation VAX 11/780 and the Prime 400). The first principal objective is to organize a body of numerical procedures in such a way that they may be invoked automatically by processes which accept symbolic and algebraic specifications from a user, and produce combined symbolic and numerical output. The second principal objective is to make the algebraic system as flexible and useful as possible in this context, and to integrate it successfully into a man machine design which provides operating system, language, and algorithm support.

UNIVERSITY OF CALIFORNIA, BERKELEY
Department of Mathematics
Berkeley, California 94720

44. ANALYTICAL AND NUMERICAL METHODS $88,844 01
Jerrold Marsden, Alan Weinstein

Stability of Elastic Systems and Plasmas

Stability and bifurcation in elasticity, fluids, and plasmas can involve both complex dynamics and stationary configurations. Such studies can be greatly facilitated by a Hamiltonian formalism. Our work falls into two areas. The first problem is a study by Chillingworth, Marsden and Wan on the number and stability of equilibrium solutions in nonlinear elasticity. This work gives a satisfactory answer to the traction problem for a body near equilibrium. Progress has recently been made on (a) the traction problem with a general reference configuration, (b) the incompressible case, and (c) the pressure problem. The methods involve the use of bifurcation theory and symmetry groups. The second problem concerns the dynamics of fluids and plasmas. Recently, Morrison, Greene, Marsden, Weinstein and others have obtained the correct Hamiltonian form for the Maxwell-Vlasov and MHD equations. We have recently developed these ideas and applied them to related systems such as the vortex models of Chorin, Beale and Majda. We hope to combine them with recent and continuing work of Holmes and Marsden which investigates chaotic dynamics and horseshoes in these equations and related systems such as the three-wave interaction model.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF COLORADO
Computer Science Department
Boulder, Colorado 80309

45. ADVANCED COMPUTING CONCEPTS $99,920 03
Lloyd D. Fosdick, Leon J. Osterweil

Software Engineering - TOOLPACK

The purpose of the Toolpack project is to supply a set of tools capable of supporting with computing power the process of creating Mathematical Software. To this end, the Toolpack project has enumerated a set of tool capabilities which it proposes to furnish. This set of capabilities includes a source code transformer, a range of static analyzers, a dynamic analyzer, a formatter, a syntax driven editor, a parser, a lexer and a number of lower level tools.

These capabilities are to be supplied as stand alone tools, and also as capabilities embedded in a larger system, called the Integrated System of Tools (IST). This larger system is in effect a programming environment for Mathematical Software. It features a very powerful language for the manipulation and management of programs under development and maintenance. This language is designed to be comfortable for users and a positive aid in marshalling the various tool capabilities effectively and efficiently. The IST architecture is centered around a file system which holds all information of interest to users and of value to the tools. The tools themselves are composed of modular tool fragments in such a way that new or altered tool capabilities can be synthesized. This renders IST a flexible and extensible environment. Toolpack is a cooperative project involving eith institutions (Argonne National Laboratory, Bell Telephone Laboratories, IMSL, Inc., Jet Propulsion Laboratory, Nag, Ltd., Purdue University, University of Arizona and the University of Colorado, Boulder). The University of Colorado is the technical coordination organization, and has carried out the sy,stems design and implementation work, as well as development of many of the tools and tool fragments.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF DELAWARE
Department of Mathematics
Newark, Delaware 19711

46. ANALYTICAL AND NUMERICAL METHODS $48,693 01
Robert Gilbert

Mathematics of Oil Production and Transportation

The subject under study is the mathematics of modeling thermal secondary oil recovery techniques, either by in situ combustion or hot water or steam injection. The study also includes inverse methods for determining the location and shape of interfacial strata between water, oil, and gas. The investigators are exploring modifications of a simplified in situ combustion model, taking into account both the oil phase and the gas phase and including the effects of gravity segregation of condensate.

Also, a systematic study of the derivation of equations that characterize the macroscopic motion of fluids in a porous elastic medium will be undertaken.

UNIVERSITY OF FLORIDA
Database Systems Research and Development Center
Department of Computer and Information Sciences
Gainesville, Florida 32611

47. INFORMATION ANALYSIS TECHNIQUES $50,000 02
Stanley Y. W. Su, Sham Navathe, Don Batory

Logical and Physical Modeling and Design of Scientific and Statistical Databases for Energy Research

In energy related research scientists often need to access diverse and interdisciplinary scientific and statistical databases (SSDs). These databases may contain energy, census, geographical, environmental, or socioeconomic data that have been gathered by different DOE laboratories or other government agencies. In general, different databases are implemented on different hardware using different data processing systems. Consequently, there are no common conventions for naming, describing, formating, representing, and structuring data. Access to data in multiple databases is thus rendered very difficult, if not impossible.

This research focuses on the logical and physical modeling and design of SSDs. The main thrusts of our current work in the logical modeling are: (1) the investigation of a powerful data model called SAM* to provide for the modeling of a variety of data types, aggregation functions and statistical summary and for the description of existing diverse databases; (2) the design of a statistical and scientific data language called SSDL that allows a statistical user who is not woo well versed in programming to perform a wide range of statistical manipulation operations; and (3) the study of the data mapping problem between a conceptual model defined by SAM* and the conceptual models defined by the existing data models. These research tasks are important and essential for the development of a powerful database management system for processing DOE-related databases.

The main thrust of our physical modeling effort is to develop a general and practical model for describing the underlying physical structures and internal operations of existing SSDs. Implementations of commercial and specialized database systems are being used as guiding references in the developoment of the model. The approach involves precise mappings from conceptual (SAM*) records (and operations on them) to actual physical records (and operations on them). Automating the development of physical database software and performance modeling packages, based on our research, will be investigated. These research tasks are essential prerequisites for modeling and improving the design and performance of current and future DOE-related databases.

40-574 O - 85 - 28

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF ILLINOIS
Computer Science Department
Urbana, Illinois 61801

48. ANALYTICAL AND NUMERICAL METHODS $220,000 01
C. W. Gear, D. S. Watanabe

Computational Mathematics - Ordinary Differential Equations

Theory, algorithms, and software for the solution of a variety of challenging problems in differential equations and their applications are being developed on this project. Among the difficult problems being investigated are those with highly oscillatory solutions, those with discontinuities, and large problems with sparse structure. We are also studying the differentiability of numerical codes for differential equations in order to develop methods with smooth solutions. Experimental software had previously been developed for the oscillatory problem and tried on a number of test problems. A production version is now being written using the extended theory of modified divided differences developed for this problem. This effort also involves writing a new integrator for standard stiff/non-stiff problems. Other software is being written for smooth integration. Methods for discontinuous problems have been incorporated in some of the earlier experimental codes and will be added to the new codes being written. Applications of numerical methods to the partial differential equations arising in semiconductor modelling are being studied. Currently we are investigating hot-electron phenomena in short-channel MOSFETs including avalanche breakdown and injection into the gate-oxide. Work is nearly complete on the hot-electron code. Additional work is underway on the development of tools for the preparation of mathematical software. In particular, we are investigating the use of Vaxima in the development of numerical software.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF ILLINOIS
Department of Computer Science
1304 West Springfield Avenue
Urbana, Illinois 61801

49. ADVANCED COMPUTING CONCEPTS $155,000 03
David Kuck, Duncan Lawrie

Design Evaluation and Use of High Performance Computer Systems

Despite the vastly improving technology available to the computer industry, there are still application areas which are beyond the capabilities of conventional computers. To get sufficient performance for these applications requires the design and construction of very high performance computers, "supercomputers", with organizations, including parallel, pipeline, and multiprocessing computers. However, programs must undergo significant changes in their structures before they can take advantage of the high performance offered by these computers.

Over the past ten years we have developed a "supercompiler", Parafrase, which analyzes Fortran programs and is capable of restructuring them to execute more efficiently on very high speed computers. The present grant funds two activities. First, the development of a computer architecture simulation facility which, together with Parafrase, will enable us to evaluate the performance of proposed new computer organizations before they are actually built. This facility includes two simulators which are currently under development. One is designed to simulate array (SIMD) computers. The other deals with multiprocessor (MIMD) organizations. This latter simulator is driven by address traces generated from programs which have been transformed by Parafrase to take advantage of multiprocessing. Both of these simulators will eventually be combined into an easy to use facility which will allow users to get performance estimates for their computers and applications programs. The second activity is to use Parafrase to analyze a number of current application programs to determine the best way to restructure them for current computers. By examining a few of these programs, we have found that they employ constructs that cause them to miss getting significant performance gains from high speed computer architectures. By using Parafrase we can identify those constructs and suggest alternatives that allow full utilization of these computers.

Using the information obtained from the above studies, we are currently specifying the organization of a new supercomputer that will be scalable to several thousand processors, each processor having performance in excess of one megaflop. Since this computer is being designed to complement a restructuring, optimizing compiler, we expect it to be easier to use than present supercomputers. By using new, very high bandwidth communication hardware, this computer will be capable of high performance on a wide variety of applications, and we expect it to be able to satisfy many of this country's more pressing computational needs in the next decade.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF MARYLAND
Department of Mathematics
Department of Electrical Engineering
Institute for Physical Science and Technology
Department of Physics and Astronomy
Laboratory for Plasma and Fusion Energy Studies
College Park, MD 20742

50. ANALYTICAL AND NUMERICAL METHODS $113,805 01
Edward Ott, James Yorke

Study of Chaotic Dynamics and the Dimension of Strange Attractors

This research is directed towards obtaining an understanding of chaotic (strange) attractors. A principal tool in this research is computer experiments. Current emphasis is on two key areas of research: (1) the dimension of chaotic attractors, and (2) the evolution of attractors as a parameter of the system is varied. The work on dimension of chaotic attractors is focused on measuring numerically the dimension of chaotic attractors and exploring the possible relations between Lyapunov numbers and the various definitions of dimension. Extensive numerical tests are applied to various dynamical systems and coupled with the information obtained from special analytically solvable maps. Investigations are also carried out concerning the utility of various definitions of dimension for estimating the information necessary to specify approximations to quantities like the distribution function on a chaotic attractor. In our second major area of research (the evolution of attractors), current emphasis has been on the study of discontinuous changes in chaotic dynamics as a system parameter is varied. Sudden changes in chaotic attractors are called crises and occur at parameter values at which the chaotic attractor collides with an unstable periodic orbit. Through numerical investigations of invertible and non-invertible maps of various dimensions, and systems of differential equations, we are investigating the characteristics of crises in typical dynamical systems. Furthermore, the statistical properties associated with crises, (e.g., the decay time of chaotic transients) are also being investigated.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF TEXAS
Department of Computer Science
Austin, Texas 78712

51. ADVANCED COMPUTER CONCEPTS $107,443 03
James Browne, G. J. Lipovski, M. Malek

High Performance Parallel Computing

This research program combines theoretical/modeling and empirically oriented approaches to varistructured and multiphased parallel formulation of computations. The thrust is not only to find and describe procedures for parallel computing but to evaluate the mechanisms and methodologies proposed by driving significant problems all the way to execution on a highly flexible parallel hardware system - the Texas Reconfigurable Array Computer (TRAC).

The prototype configuration of TRAC consists of 16 processors and 91 TRAC provides varistructure and resource partitioning, which support memories-I/O units, scheduled to be operational in the Fall of 1982. the concept of designing an architecture for an algorithm rather than mapping an algorithm to an architecture. The TRAC interconnection network implements processor-memory and processor-processor circuits and also a high performance packet switching capability. This allows study of process execution models ranging from pure shared memory intercommunication to completely disjoint and distributed address spaces.

There are three principal research areas: software for varistructured reconfigurable multiprocessor architectures, multi-phase parallel formulation of significant complete problems, and further development of the varistructure reconfigurable network based computer architectures.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF TEXAS
Texas Institute for Computational Mechanics
Austin, Texas 78712

52. ANALYTICAL AND NUMERICAL METHODS $92,738 01
Graham F. Carey, David M. Young

Iterative Solution and Finite Element Analysis
in Computational Mechanics

This research concerns the use of iterative solution algorithms in conjunction with finite element methods for computing numerical solutions of transient and nonlinear problems in mechanics and heat transfer. Particular focus is directed towards the solution of very large scale, complex problems by means of advanced computer architectures exploiting vectorization and parallelism.

In the theoretical and numerical investigations we examine accuracy and error estimates for certain classes of transport problems - for example, in heat transfer, reservoir simulation, and Navier-Stokes theory. Related interesting questions concerning special techniques, such and "lumping" and "upwinding" are being examined. Moreover, we seek to determine the influence of such strategies on the structure and behavior of the approximate problem and solution iterative techniques.

The analysis of transient problems is based on a semidiscrete formulation in which selection of appropriate system integrators play an important part in determining the overall efficiency of the computation. In the investigation of iterative techniques we study the properties of the methods for the classes of problems indicated, acceleration of the methods and tailoring specific methods to exploit special features of emerging computer architectures of current interest. Numerical case studies will help provide an evaluation of the technical innovations arising from the study of finite element and iteration methods.

UNIVERSITY OF UTAH
Department of Mathematics
Salt Lake City, Utah 84112

53. INFORMATION ANALYSYS TECHNIQUES $1.9,684 02
Robert Barnhill

Computer Aided Surface Representation and Design

This research creates new methods for representing and approximating three and four dimensional surfaces. These schemes are the core of our forthcoming Surface Software Package. Surfaces can be understood adequately only through the use of dynamic computer graphics; therefore, graphics capability is also included. The numerous applications of surface methods include modeling physical phenomena (e. g., combustion) and designing objects (e. g., airplanes and cars). In addition to three dimensional surfaces, there are interesting four dimensional "surfaces," such as temperature as a function of the three spatial variables. Because the geometric information for these problems can be located arbitrarily in three or four dimensional space, the surface schemes must be able to handle arbitrarily located data. The standard (and easier) approach to surfaces of using tensor products of curve methods restricts the surface method's applicability to (rectangularly) "gridded" data. We take the more ambitious approach of devising robust surface methods applicable to arbitrarily located data. There are two broad classes of methods suitable for solving these problems (i. e., problems for which simplifying geometric assumptions cannot be made):

(1) surface interpolants defined over triangles or tetrahedra

(2) surface interpolants defined directly from the given data.

Users ordinarily want smoother surfaces than their data imply directly, so that additional information must sometimes be created. (A notable feature of our methods is that the smoothness of the surface is always greater than or equal to the smoothness of the data. This is not true of most other schemes such as finite element schemes.) Rendering three and four dimensional surfaces in a form maximally useful to the user is another interesting and difficult problem. We are using interactive computer graphics to display three dimensional surfaces and will add color to help visualize and interpret four dimensional surfaces.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF WASHINGTON
Applied Mathematics Program
Seattle, WA 98195

54. ANALYTICAL AND NUMERICAL METHODS $37,785 01
Jirair Kevorkian

Resonance in Weakly Nonlinear Systems

Resonance is a common phenomenon in any physical process that involves coupled oscillations. In this research project some recent work on nonlinear resonance in systems with slowly varying frequencies is studied and the application of this work to a quantitative description of the operation and stability of free electron lasers is being investigated. Progress in deriving adiabatic invariants for systems passing through resonance is sought and work on wave propagation problems using multiple variable expansion techniques is planned. New research in planned in the following areas:

(1) A systematic analysis of free electron lasers, including higher order effects and stability;

(2) A study of nonlinear evolution equations as they occur in the analysis of free electron lasers or more generally in systems with strong interactions between modes;

(3) The influence of nonlinear dissipations; and

(4) Resonant wave interactions in unbounded media with slowly varying properties.

This project is a new start in FY 1983.

DOE Applied Mathematical Sciences FY 1983

UNIVERSITY OF WISCONSIN
Computer Science Department and
Statistics Department
Madison, Wisconsin 53706

55. INFORMATION ANALYSIS TECHNIQUES $94,937 02
David J. DeWitt, Computer Sciences Department
Doug Bates, Statistics Department

Database Machines for Large Statistical Databases

This project deals with the investigation of database machines for supporting efficient access to large statistical databases. Most, if not all, database machine designers have concentrated on the efficient support of operations on relational databases. This project is examining how analysis of very large data sets can be enhanced through specialized hardware and software.

To achieve this objective a number of related problems are being addressed. First the way in which statisticians access and manipulate their data sets has led to the design of a database system organization that facilitates the statistical analysis of very large data sets. The key components of the proposed system include concrete views of the raw database for each analyst, a Summary Database for each view that automatically maintains the results of a number of system and analyst defined functions while the view is being edited, and a Management Database that is used for maintaining definitions of new functions and the history of changes that have been made to each view (including a specification of the operations that were utilized to materialize the view).

Another component of the present research project has been the development of a set of fundamental building blocks which a statistical database machine should support as its "machine language." Examination of a large number of algorithms for statistical operations revealed that these algorithms can be implemented by using a relatively well defined set of linear algebra operations. Presently we are evaluating uniprocessor algorithms and alternative storage organization for this set of building blocks. The next step is to design a number of parallel algorithms and to implement a prototype statistical database machine using these building blocks. Examination of the performance of this prototype system will be used to gather information about the suitability of our building blocks. This information, along with parameters characterizing various mass storage systems, storage organizations, and compression techniques will then be used to evaluate alternative parallel algorithms for each building block. The final step will be to design a high performance statistical database machine that permits the efficient execution of the algorithms selected.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY
Laboratory for Transport Theory
and Mathematical Physics
Blacksburg, Virginia 24061

56. ANALYTICAL AND NUMERICAL METHODS $48,280 01
William Greenberg, P. F. Zweifel

Applied Mathematics of Transport Theory

During the past twelve months research has continued on several projects. These can be classified into five general areas -- Existence Theory for the Nonlinear Boltzmann Equation; Transport Theory; Gas Dynamics; Plasma Stability; and miscellaneous topics. Explicit results include an existence proof for the Boltzmann equation with unbounded collision kernels; existence proofs for a generalized version of the linear transport equation with an unbounded collision type operator; an improved iteration scheme for numerical solutions of the transport equation; construction of solutions to the linearized BGK equations of two component gas flow; nonlinear stability of asymptotic suction; and stability of the nonlinear Vlasov equation, with special attention to the interaction between the linear eigenvalue and the Case-van Kampen continuum. Studies are continuing in many of these areas. Ongoing studies include general theorems for Weiner-Hopf factorization of infinite matrices (i. e., operators in L2) based on the existence theory for the generalized transport equation mentioned above, and detailed analysis (including numerics) of the influence of continuum modes on a nonlinear plasma stability (perturbation of the equilibrium distribution).

YALE UNIVERSITY
Computer Science Department
New Haven, CT 06520

57. ANALYTICAL AND NUMERICAL METHODS $48,693 01
Tony F. C. Chan

Numerical Methods for Nonlinear Elliptic Eigenvalue Problems

Nonlinear eigenvalue problems are problems of the form G(u,p)=0, where u belongs to some Banach space and p is a scalar parameter. Many important problems in the physical sciences can be cast in this form. Among these are problems in elasticity, structural mechanics, fluid dynamics, chemical engineering, meteorology, and plasma physics. These problems often possess interesting nonlinear bifurcation phenomena, for example, the existence of limit points and bifurcation points.

The ultimate objective of this project is to produce efficient and reliable software for such problems. We are investigating both the numerical and software aspects that arise. The basic method we are using is the arclength continuation method of H. B. Keller. Among some of the important computational issues are: fast location of singular points, automatic step size algorithms, improvement of the basic Newton process and fast linear algebra solution methods for large elliptic problems. A software package is being developed.

List of Investigators

Albright, N.	26
Amos, D. E.	58
Barnhill, R.	72
Bates, D.	74
Batory, D.	66
Beauchamp, J. J.	51
Berger, M. J.	36, 46
Betancourt, O.	36, 43
Bianchini, R.	48
Bjorstad, P.	36, 44
Bountis, T.	17
Bowman, K. O.	51
Boyle, J. M.	10
Browne, J.	70
Bryant, R.	15
Bucher, I.	25
Burnett, R. A.	53
Butler, T. D.	24
Buzbee, B.	25
Carey, G. F.	71
Carlson, B.	08
Carlson, R.	30
Carr, D. B.	53
Chan, T. F. C.	76
Chorin, A. J.	26
Clayton, R.	15
Cody, W. J.	09
Colella, P.	26
Coleman, T. F.	18
Concus, P.	26
Corones, J.	08
Cottle, R. W.	60
Cowell, W. R.	10
Cowley, P. J.	53
Dantzig, G. B.	60
Davison, M.	08
DeWitt, D. J.	74
Dennis, J. B.	33
Dennis, J. E.	56
Dongarra, J. J.	09, 10
Dritz, K. W.	10
Erickson, M. D.	53
Fasel, J.	25
Fateman, R. J.	62
Feigenbaum, M. J.	19 ,24
Fogelson, A.	26
Foias, C.	21
Foley, J. D.	20
Fosdick, L. D.	64
Fox, G. C.	15
Franceschini, E.	49

Frederickson, P. 25
Fredkin, E. 34
Fritsch, F. 30
Funderlic, R. E. 50
Gabriel, J. R. 10
Garbow, B. S. 09
Gauteson, A. K. 08
Gear, C. W. 67
Gelinas, R. J. 57
Gilbert, R. 65
Glimm, J. 36, 43
Goldstein, C. 13
Goldstein, M. 49
Golub, G. H. 61
Goodman, J. 36, 47
Gray, L. J. 50
Greenberg, W. 75
Greiman, W. 28
Grumbaum, F. A. 26
Hager, B. 15
Hald, O. H. 26
Hall, D. L. 53
Harten, A. 36, 44
Hawthorn, P. 27
Heath, D. 36, 40
Heath, M. T. 50
Hillstrom, K. E. 09
Hindmarsh, A. 30
Hiromoto, R. 25
Hyman, J. M. 24
Isaacson, E. 36, 45
Jordan, T. 25
Kahan, W. 62
Kalos, M. H. 36, 38-41, 48
Kao, C. S. 14
Kaper, H. G. 09
Kee, R. J. 59
Keller, H. B. 15, 16
Kevorkian, J. 73
Krueger, R. 08
Kuck, D. 68
Kupperman, A. 15
Lawrie, D. 68
Lax, P. D. 36
LeVeque, R. 36, 47
Leaf, G. K. 09
Lebowitz, J. 36, 39, 41
Lipovski, G. J. 70
Littlefield, R. J. 53
Lusk, E. 10
Lyness, J. N. 09
Majda, A. 26
Malek, M. 70

Margolis, S. 59
Margolus, N. 34
Marr, R. 13
Marro, J. 36
Martin, A. 15
Marsden, J. 63
Matkowsky, B. J. 09, 35
McBryan, O. 36, 43
McGraw, J. 31
McMaken, H. 08
Messina, P. C. 09-11
Michael, G. 30, 31
Mickens, R. E. 12
Minkoff, M. 09
Mitchell, T. J. 51
More', J. J. 09
Morris, M. D. 51
Murray, W. 60
Nanda, T. 26
Navathe, S. 66
Nichols, B. 24
Nicholson, W. L. 53
Nocedal, J. 36, 42
O'Dell, M. 28
Osterweil, L. J. 64
Ott, E. 69
Overbeek, R. 10
Overton, M. L. 36, 41, 42
Pasciak, J. 13
Peierls, R. 14
Percus, J. 36, 40
Peskin, C. S. 36, 37
Petzold, L. R. 59
Quong, C. 27, 29
Rice, J. R. 55
Robbins, H. 14
Rodrique, G. 31
Saffman, P. G. 15, 16
Salama, M. 15
Schwartz, J. T. 48
Seitz, C. L. 15
Sethian, J. A. 26
Shampine, L. F. 58
Shoshani, A. 27
Siggia, E. D. 19
Skinner, D. 38
Smith, B. T. 10
Smooke, M. 59
Solomon, A. D. 50
Sorensen, D. C. 09
Stewart, H. 13
Su, S. Y. W. 66
Sventek, J. 28

Tabor, M. 23
Tapia, R. A. 56
Thomas, J. J. 53
Toffoli, T. 34
Trefethen, L. N. 36, 46
Tsai, W.Y. 14
Tukey, J. 54
Varga, R. S. 22
Vichniac, G. 34
Wang, P. S. 22
Ward, R. C. 50-52
Watanabe, D. S. 67
Weinstein, A. 63
Weiss, J. 23
Whitlock, P. A. 36, 38, 39
Widlund, O. 36, 44, 45
Wilson, D. G. 50, 52
Wos, L. T. 10
Wright, T. 51
Yorke, J. A. 69
Young, D. M. 71
Zettl, A. 09
Zweifel, P. F. 75
van Ryzin, J. 14

H. Engineering Research Program

1. What is the detailed budget structure of the Engineering Research Program? What types of work are funded by each of these budget categories?

Answer: The Engineering Research Program budget is divided into three categories:

- Mechanical Sciences--including tribology (basic nature of the phenomena of friction, wear and tear), heat transfer by conduction, convection, and/or radiation, fluid mechanics, and solid mechanics with emphasis on continuum mechanics and crack propagation.

- Systems Sciences--including intelligent controls for energy related plants, analysis of total systems and component interactions with the application of the theory of control and decision, and the research and development of appropriate instrumentation and apparatus for energy applications.

- Engineering Data and Analysis--including the study of the motion of and interaction among complex physical systems (non-linear dynamics), development of data bases for thermophysical properties of fluids and fluid mixtures, and modeling of combustion processes for engineering applications.

2. For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.

Answer:

B/A
$ in Millions

	FY 1981	FY 1982	FY 1983	(Estimated) FY 1984	FY 1985
Mechanical Sci (MS)					
OE	1.5	1.5	1.7	1.8	2.0
CE	0	0	0.1	0	0.1
Sys. Sci. (SS)					
OE	1.0	1.4	2.1	2.4	3.0
CE	0.1	0.2	0	0.1	0.3
Eng. Data & Analysis (EDA)					
OE	0.9	1.0	1.5	2.1	2.1
CE	0	0	0.1	0.1	0
Total					
OE	3.4	3.9	5.3	6.3	7.1
CE	0.1	0.2	0.2	0.2	0.4

3. For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Engineering Research funding going to DOE laboratories.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
ENGINEERING, MATHEMATICAL AND GEOSCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC04 ENGINEERING, MATHEMATICAL AND GEOSCIENCES					
KC0401 ENGINEERING SCIENCES					
KC0401010 TRIBOLOGY					
OPERATING EXPENSES					
OAK RIDGE NATIONAL LAB	$ 75	$ 0	$ 0	$ 0	$ 0
KC0401020 HEAT TRANSFER AND HEAT EXCHANGERS					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	0	30	100	120	130
PACIFIC NORTHWEST LABS	100	100	125	135	0
KC0401030 GEOSCIENCES					
OPERATING EXPENSES					
AMES LAB	100	150	200	200	250
ARGONNE NATIONAL LAB	0	0	0	50	110
IDAHO NATIONAL ENG LAB	40	50	45	110	120
LAWRENCE LIVERMORE NAT LAB	130	0	250	160	100
LOS ALAMOS NATIONAL LAB	50	0	160	175	200
OAK RIDGE NATIONAL LAB	0	0	200	400	450
PACIFIC NORTHWEST LABS	60	50	0	0	0
SANDIA CORP	75	45	100	110	120
KC0401040 SOLID MECHANICS					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	45	50	0	0	0
IDAHO NATIONAL ENG LAB	90	100	155	165	175
KC0401050 THERMOPHYSICAL PROPERTIES OF FLUIDS AND COMBUSTION ENGINEERING					
OPERATING EXPENSES					
LAWRENCE BERKELEY LAB	127	150	160	180	190
SANDIA LAB, LIVERMORE	100	100	150	160	170

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0401060 ENGINEERING ANALYSIS					
OPERATING EXPENSES					
LAWRENCE BERKELEY LAB	50	75	90	100	120
CAPITAL EQUIPMENT					
AMES LAB	40	20	25	30	20
ARGONNE NATIONAL LAB	0	50	10	0	0
IDAHO NATIONAL ENG LAB	28	0	40	20	50
LAWRENCE BERKELEY LAB	36	0	40	40	40
LAWRENCE LIVERMORE NAT LAB	10	0	0	0	0
OAK RIDGE NATIONAL LAB	0	0	15	90	250
PACIFIC NORTHWEST LAB	10	0	0	10	0
SANDIA LABS	8	30	0	0	20

4. **For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of Engineering Research funding going to universities.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
ENGINEERING RESEARCH PROGRAM
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0401 ENGINEERING SCIENCES					
KC0401010 TRIBOLOGY					
OPERATING EXPENSES					
ARIZONA UNIV OF	$ 4	$ 0	$ 0	$ 0	$ 0
COLORADO SCHOOL MINES	0	- 2	0	0	0
COLORADO UNIV OF	5	0	0	0	0
ILLINOIS INST TECH	0	79	80	0	0
MASSACHUSETTS INST TECH	150	125	35	80	150
MICHIGAN UNIV OF	67	0	0	60	75
KC0401020 HEAT TRANSFER AND HEAT EXCHANGERS					
OPERATING EXPENSES					
CALIF UNIV OF LOS ANGELES	0	55	61	66	0
CALIF UNIV OF SANTA BARBARA	0	0	0	40	0
CLARKSON COLLEGE OF TECH	0	66	69	75	0
COLORADO SCHOOL MINES	40	45	0	0	0
ILLINOIS UNIV OF	40	53	0	0	0
IOWA UNIV OF - IOWA CITY	55	0	0	0	0
MARYLAND UNIV OF	35	40	18	0	50
MASSACHUSETTS INST TECH	0	54	60	30	0
MINNESOTA UNIV OF	65	72	151	168	190
NORTHWESTERN UNIV	51	50	0	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
PENNSYLVANIA STATE UNIV	8	10	- 5	0	0
STANFORD LELAND JR UNVR	70	73	130	49	152
VIRGINIA POLYTECHNIC INST	0	59	94	100	101
KC0401030 GEOSCIENCES					
OPERATING EXPENSES					
BROWN UNIV	81	96	0	0	0
CORNELL UNIV	0	115	115	80	0
ILLINOIS INST TECH	53	74	0	120	100
MASSACHUSETTS INST TECH	115	45	149	224	270
MASSACHUSETTS UNIV OF	59	65	0	70	160
NORTHWESTERN UNIV	0	0	53	55	59
PENNSYLVANIA UNIV OF	0	100	100	75	25
STANFORD LELAND JR UNVR	114	158	97	0	110
WISCONSIN UNIV OF	100	130	80	90	230
KC0401040 SOLID MECHANICS					
OPERATING EXPENSES					
ILLINOIS UNIV OF	0	0	39	41	43
PENNSYLVANIA UNIV OF	0	0	69	67	0
RUTGERS UNIV	45	33	0	0	0
STANFORD LELAND JR UNVR	61	152	216	136	355
KC0401050 THERMOPHYSICAL PROPERTIES OF FLUIDS AND COMBUSTION ENGINEERING					
OPERATING EXPENSES					
BRIGHAM YOUNG UNIV	0	0	0	20	60
BROWN UNIV	20	0	103	70	0
CARNEGIE MELLON UNIV	50	0	0	0	0
COLORADO SCHOOL MINES	0	0	80	40	40
CORNELL UNIV	0	0	42	22	34
MASSACHUSETTS INST TECH	0	0	130	140	165
NORTHWESTERN UNIV	0	0	0	70	0
RICE WILLIAM MARSH UNIV	0	41	20	0	0
KC0401060 ENGINEERING ANALYSIS					
OPERATING EXPENSES					
BROWN UNIV	0	0	0	70	85
CALIF UNIV OF SAN DIEGO	0	0	0	50	0
CHICAGO UNIV OF	85	95	105	115	125
CORNELL UNIV	0	0	0	3	0
MARYLAND UNIV OF	0	0	0	50	0
MASSACHUSETTS INST TECH	68	0	0	0	0
MINNESOTA UNIV OF	0	0	50	70	75
NEW YORK CITY UNIV	200	200	260	150	250
ROCKEFELLER UNIV	79	61	53	0	80
SOUTHERN CAL UNIV OF	0	0	63	70	0
STANFORD LELAND JR UNVR	0	45	92	97	150
STEVENS INST OF TECH	0	0	0	40	0
TEXAS UNIV OF	100	100	82	98	120
WEST VIRGINIA UNIV	0	0	0	83	0

5. **For the period FY 1981 - FY 1985, please provide, by budget category and by company, the amount of Engineering Research funding going to industry.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
ENGINEERING RESEARCH PROGRAM
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0401 ENGINEERING SCIENCES					
KC0401010 TRIBOLOGY					
OPERATING EXPENSES					
CALSPAN CORPORATION	$ 98	$ 110	$ 117	$ 0	$ 0
ELECTROCHEMICAL TECH. CORP.	0	0	69	66	83
SKF INDUSTRIES	119	0	0	0	0
KC0401020 HEAT TRANSFER AND HEAT EXCHANGERS					
OPERATING EXPENSES					
BIPHASE ENERGY SYSTEMS	65	63	0	0	0
CALSPAN CORPORATION	70	62	0	0	0
FLOW INDUSTRIES INC	0	0	0	60	0
GENERAL ATOMIC CO	0	75	95	100	25
KC0401030 GEOSCIENCES					
OPERATING EXPENSES					
SCIENTIFIC SYSTEMS	0	0	25	0	48
SYSTEMS ENG. POWER, INC.	60	62	0	0	0
KC0401040 SOLID MECHANICS					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	43	0	56	56	56
T.S. ASSOCIATES, INC.	58	0	0	0	0
KC0401060 ENGINEERING ANALYSIS					
OPERATING EXPENSES					
GEOCHEM RESEARCH	0	100	21	109	69
PHYSICAL SCIENCES, INC.	0	0	0	60	0
SCIENCE APPLICATIONS	0	0	0	72	0
SKF INDUSTRIES	0	0	0	100	125

6. **How does the research funded by the Engineering Research Program differ, complement, supplement, or overlap engineering research funded by other DOE programs and by other agencies such as the National Science Foundation?**

Answer: The Engineering Research Program strives to identify and support fundamental research on broad, generic topics in engineering sciences with particular emphasis on problems related to energy production, distribution and utilization. Broader in application and of greater generic value engineering research is distinct from research sponsored by the Department's technology programs which have more specific, short term objectives. In the Engineering Research Program, special emphasis is placed on projects whose successful conclusion is likely to affect more than one energy technology. To cite an example, an understanding of the basic principles underlying the flow of multiphase fluids (mixtures of fluids at both gaseous and liquid phases) is required for the solution of many problems in petroleum and chemical industrial processes as well as in specific energy systems: geothermal, chemical energy, solar energy, etc. State-of-the-art instrumentation and apparatus for use in extreme environmental conditions (high temperatures, high pressures and hazardous conditions) are valuable in many energy systems. In contrast, technology programs support research directed at the solution of more narrowly defined technical problems within their immediate purview.

In contrast with the National Science Foundation's Engineering Program, the DOE Engineering Research Program has its priorities established first and foremost by the Department's mission requirements. Thus, while the NSF Program funds problems of general interest, the DOE Program funds research principally in energy-related engineering areas, with higher education playing an important but not dominant role.

7. **What types of formal and informal advisory groups does the Division of Engineering and Geosciences to assure that the Engineering Research Program is of high quality and coordinated with the research carried out at other agencies? If any formal advisory groups exist, please provide a listing of the current membership.**

Answer: The Engineering Research Program has no chartered formal or informal advisory committee. Interagency coordination is maintained through direct personal contacts with program managers in the other agencies. The quality is assured by peer review of individual proposals and external site review panels when appropriate. The Council on Energy Engineering Research assists the Engineering Research Program in selecting areas of research for review. Ad hoc technical reviews of specific research areas are undertaken as needed, while workshops are held to stimulate individual contributions at the frontiers of engineering research. The Council is an outgrowth of earlier activities in ERDA and DOE aimed at stimulating ideas in areas deemed important for the future. It consists of engineering researchers from academia, industry and DOE laboratories.

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8. **There has been a growing concern expressed by professional engineering groups, universities, and advisory groups that a higher national priority be placed on engineering research. What particular areas of national importance do you believe should be addressed in an enhanced Engineering Research Program?**

Answer: A number of energy related areas have been identified with the help of several workshops and discussions with individual leading members of the engineering research community. The Department of Energy is not proposing

enhancement of the BES Engineering Research Program, but the workshops and discussions provide guidance helpful in program implementation. The principal areas being discussed are:

1) Intelligent controls and self repairing mechanisms--needed for servicing and maintaining future advanced energy systems with local environment potentially dangerous to human beings, e.g. nuclear reactor containment vessels, synfuel plants, waste processing and the like.

2) Advanced methods and processes--aimed at improved energy utilization, including research on multi-phase flows, data bases, and instrumentation and control systems for plasma engineering.

3) Instrumentation--including high longevity sensors and control systems for reliable and accurate operation in hostile environments, e.g. high temperature, high pressure, chemically active or radioactive environments.

4) Structural failure control--to help reduce the cost of design, construction, maintenance, and inspection of energy systems by improvements in weldments, life-time prediction, risk and reliability analysis, and accuracy of fracture-sensitive flaw detection.

9. **How would an enhanced Engineering Research Program fit within the mission of DOE as contrasted with the Department of Commerce, the Department of Interior, the Department of Defense, etc.?**

Answer: The Engineering Research Program addresses principally those research topics which are seen as vitally important to ensuring the nation's energy well-being, which is DOE's mission. Other mission oriented Departments do not have the mandate to address the problems of prime importance to DOE; i.e., energy related problems. As noted in the response to the previous questions, the Department of Energy is not proposing enhancement of the BES Engineering Research Program.

10. **What has DOE done towards planning an enhanced Engineering Research Program?**

Answer: The planning has been focused on program effectiveness rather than enhancement. The Engineering Research Program plan follows within the available means the recommendations of a series of workshops held in 1978-79 to identify research priorities for the then newly initiated engineering program. Following an initial scoping workshop, subsequent workshops dealt with specific high priority topical areas, such as instrumentation and control systems, advanced industrial processes, fluid dynamics and thermal processes.

11. **What funding levels would be required to conduct such an enhanced Engineering Research Program?**

Answer: As noted DOE is not proposing enhancement. The BES Engineering Research program strives to cover within the available budgets as many of the high priority areas as possible.

12. How would DOE go about building an enhanced Engineering Research Program of, say, $50 million?

Answer: At present there is no detailed long range plan for an enhanced Engineering Research Program. To develop such a plan it is necessary to convene workshops and ad hoc technical panels which would identify the existing research frontiers and opportunities for important advances in the given engineering research fields.

13. How would this enhanced program differ or relate to the National Science Foundation Engineering Research Program?

Answer: Since enhancement is not being proposed, these comments will assume a level of effort near the present one. The Engineering Research Program aims to attain the goals established by the community of engineering sciences experts at the 1978 Scoping Workshop. The program is oriented towards DOE's specific mission requirement and along with frequent contacts between program managers, the DOE avoids duplicating the efforts of the National Science Foundation.

14. What would be the roles of the DOE Laboratories, universities, and industry in such an expanded program?

Answer: The present program permits some participation by research engineers and scientists from all sectors: DOE Laboratories, universities, and industry. Unsolicited proposals from these sectors would continue to be the primary method for funding such research.

15. Are there opportunities to utilize national technical resources at both DOE Laboratories and at universities in a coordinated collaborative fashion to address engineering research problems?

Answer: At present there are several such opportunities:

1) The Center for Engineering Science Advanced Research (CESAR) at ORNL has started a program on intelligent controls and self-repairing mechanisms to be complemented by related activities at various U.S. universities, including especially the University of Tennessee, Stanford University and Harvard University.

2) Idaho National Engineering Laboratory and MIT are preparing a joint proposal in the fields of plasma engineering, welding and structural failure control.

3) Argonne National Laboratory offers a range of opportunities for collaboration with universities in the areas of heat transfer, multiphase flow, and continuum mechanics research.

16. Please provide a copy of the latest Engineering Research summaries.

Answer: A copy of the requested material is attached.

DOE/ER-0158/1
Dist. Category UC-38

Summaries of FY 1983 Engineering Research

December 1983

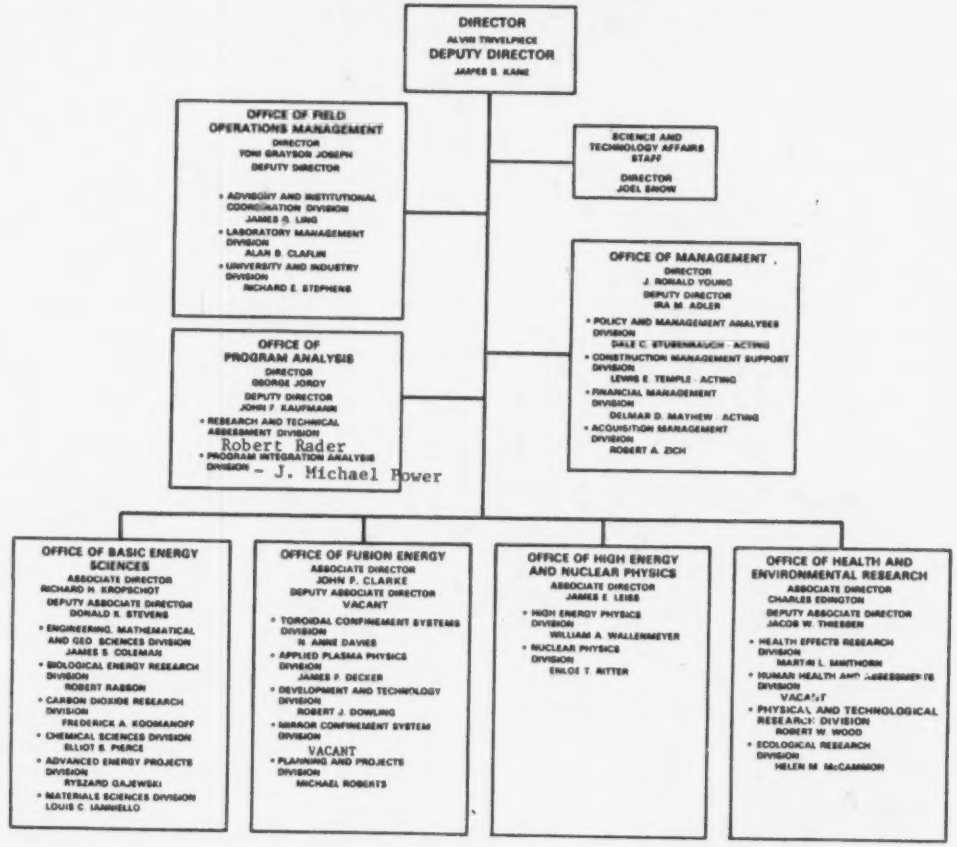
U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering, Mathematical
and Geosciences
Washington, D.C. 20545

FOREWORD

This report documents the BES Engineering Research program for fiscal year 1983; it provides a summary for each of the program projects in addition to a brief program overview. The report is intended to provide staff of Congressional committees, other executive departments, and other DOE offices with substantive program information so as to facilitate governmental overview and coordination of Federal research programs. Of equal importance, its availability facilitates communication of program information to interested research engineers and scientists. The organizational chart for the DOE Office of Energy Research (OER) on the next page delineates the six Divisions within the OER Office of Basic Energy Sciences (BES). Each BES Division administers basic, mission oriented research programs in the area indicated by its title. The BES Engineering Research program is one such program; it is administered by the Engineering, Mathematical and Geosciences Division of BES. Dr. Oscar P. Manley is technical manager of the Engineering Research program; inquiries concerning the program may be addressed to him, in writing or by phone at (301) 353-5822.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1983. The summaries received have been edited as necessary, but the press for timely publication made it impractical to have the investigators review and approve the summaries prior to publication. For more information about a given project, it is suggested that the investigators be contacted directly.

OFFICE OF ENERGY RESEARCH



INTRODUCTION

The individual project summaries follow the program overview. The summaries are ordered alphabetically by name of institution and so the table of contents lists all of the institutions at which projects were sponsored in fiscal year 1983.

The projects are numbered sequentially for individual identification in the indexes. Each project entry begins with a centered, institutional-departmental heading. The project number precedes the capitalized project title. The names of the investigators are listed immediately below the title. The funding level for fiscal year 1983 appears to the right of the title; it is followed by the budget activity number (e.g., 01-03). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The year in which the project began and the anticipated duration in years are indicated respectively by the first two and last digits of the sequence directly below the budget activity number (e.g., 80-2). The summary description of the project completes the entry.

TABLE OF CONTENTS

	Page
Program Overview	1
Project Summaries	6
Ames Laboratory	6
Argonne National Laboratory	7
Arvin/Calspan	8
Battelle Columbus Laboratories	9
Biphase Energy Systems	10
Brown University	11
University of California/LA	12
Calspan Advanced Technology Center	13
University of Chicago	14
Clarkson College of Technology	15
Colorado School of Mines	16
Cornell University	18
Electrochemical Technology Corp.	20
General Atomic Company	21
Geo-Chem Research Associates	22
Idaho National Engineering Laboratory	23
University of Illinois at Urbana-Champaign	25
Illinois Institute of Technology	27
Jet Propulsion Laboratory	29
Lawrence Berkeley Laboratory	31
Lawrence Livermore National Laboratory	33
Los Alamos National Laboratory	34
University of Maryland	35
University of Massachusetts	36
Massachusetts Institute of Technology	37
University of Minnesota	42
National Bureau of Standards	44
City University of New York	46
Northwestern University	47
Pacific Northwest Laboratory	49
University of Pennsylvania	50
Rice University	52
Rockefeller University	53
Rutgers University	54
Sandia National Laboratories	55
Scientific Systems, Inc.	57
SKF Industries, Inc.	58
University of Southern California	59
Stanford University	60
Systems Engineering For Power, Inc.	66
University of Texas at Austin	67
Virginia Polytechnic Institute and State University	68
University of Wisconsin	69
Budget Number Index	70
Project Titles	72

BES ENGINEERING RESEARCH

The BES Engineering Research program is one of the component research programs which collectively constitute the DOE Basic Energy Sciences program. The DOE Basic Energy Sciences program supports energy related reseach in the physical and biological sciences, engineering, and applied mathematics. The chief purpose of the DOE Basic Energy Sciences program is to provide the fundamental scientific base on which identification and development of future, national energy options will depend. The major product of the program becomes part of the body of data and knowledge upon which the applied energy technologies are founded; the product is knowledge relevant to energy exploration, production, conversion and use.

The BES Engineering Research program was started in 1979 to help resolve the numerous serious engineering issues arising from efforts to meet U.S. energy needs. The program supports fundamental research on broad, generic topics in energy related engineering--topics not as narrowly scoped as those addressed by the shorter term engineering research projects sponsored by the various DOE technology programs. Special emphasis is placed on projects which, if successfully concluded, will benefit more than one energy technology. During the first year several workshops were sponsored for the purpose of identifying energy related engineering research needs and initial priorities. Representatives from industry, academic institutions, national laboratories, and leading members of professional organizations (Engineering Societies Commission on Energy, American Society of Mechanical Engineers, Society of Automotive Engineers, and Joint Automation and Control Committee) participated in the workshops. In addition to the participants in the workshops, staff representatives from the DOE technology programs and other leading U.S. energy engineering experts made significant contributions to the setting of program priorities. There resulted from this process a strong confirmation of the need for a long-range, fundamental engineering research program with two major goals. The broad goals that were established by this process for the BES Engineering Research program are:

1) To extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and

2) To broaden the technical and conceptual base for solving future engineering problems in the energy technologies.

In this process, it was further established that to achieve these goals, the BES Engineering Research program should address the following topics identified as essential to the progress of many energy technologies:

1) Advanced Industrial Technology -- improvement of energy conversion and utilization, opening new technological possibilities, and improvement of energy systems.

2) Fluid Dynamics and Thermal Processes -- broadening of understanding of heat transfer in non-steady flows, methodology for reducing vibrations and noise in heat exchangers, and engineering aspects of combustion.

3) Solid Mechanics -- continuum mechanics and crack propagation in structures.

4) Dynamics and Control of Processes and Systems -- development and use of information describing system behavior (system models), performance criteria, and theories of control optimization to achieve the best possible system performance subject to known constraints.

In addition to the above topics, Geotechnical Engineering (mining), Electric Power Technology, Reliability and Risk Analysis, and Novel Energy Related Engineering were endorsed as areas suitable for immediate initiation of engineering research projects. Because of budgetary limitations, the implemented BES Engineering Research program is somewhat less broad than the program envisioned above. At present, equal emphasis is being placed on three carefully selected, high priority research areas; namely,

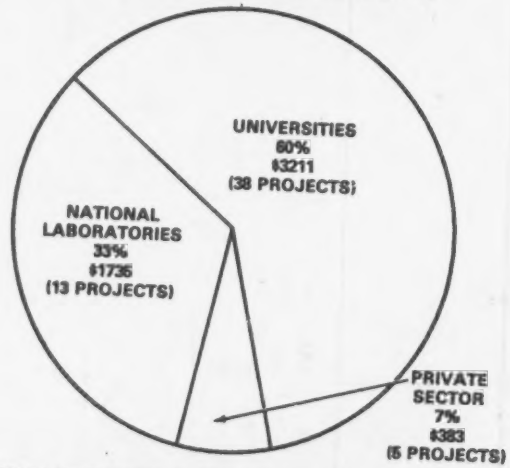
1) Mechanical Sciences -- including tribology (basic nature of friction reduction phenomena), heat transfer, and solid mechanics (continuum mechanics and crack propagation).

2) System Sciences -- including process control and instrumentation.

3) Engineering Analysis -- including non-linear dynamics, data bases for thermophysical properties of fluids, and modeling of combustion processes for engineering application.

These areas contain the most critical elements of the four topics enumerated above; as such, they are of importance to energy technologies both in the short and long term, and therefore of immediate programmatic interest. It should be noted that other areas of basic research important to engineering are monitored elsewhere in BES. For instance, fluid mechanics, especially turbulence and research on thermophysical properties, are among the responsibilities of the Chemical Sciences Division, while microscopic aspects of fracture mechanics are in the domain of the Material Sciences Division. As resources permit, other high priority areas are being added to the Engineering Research program. Thus in fiscal year 1983, a significant portion of the real increment in available funds will be used to fill a widely perceived gap between research on advanced control systems and the developments in artificial intelligence as they apply to energy systems. Further in the future as funds become available, the program will address the development of methodologies for simulating the scale-up of process plants. With the availability of an increasing data base, new concepts in the mathematical theory of non-linear systems offer opportunity for rapid advances in this relatively unexplored engineering field. Research projects sponsored by the BES Engineering Research program are currently underway at universities, private sector laboratories, and DOE national laboratories. In fiscal year 1982 the program operating funds available amounted to about $4 million. The distribution of these funds among various institutions and by topical areas is illustrated on the next page. Project funding levels are mostly in the range of $50,000 to $100,000 per year. Typical duration of a project is three to four years, with some projects expected to last as long as ten years or more. The BES Engineering Research projects stem almost without exception from unsolicited proposals. Proposals which anticipate definite results in less than two years are usually referred to the appropriate DOE technology program for consideration. Anyone interested in submitting a proposal is encouraged to discuss his ideas with the technical program manager prior to submission of a formal proposal. Such discussion helps to establish whether or not a potential project has a reasonable chance of being funded. The primary considerations for possible support are the technical quality of the proposal and the professional standing of the principal investigators and staff. An effort is made to attract first rate, younger research engineers and energy oriented applied scientists. A high technical caliber of research is maintained by requiring that the projects supported have potential for a significant contribution to energy-related engineering science, or for an initial contribution to a new energy relevant technology. Sponsored projects are selected primarily for their relevance to DOE mission requirements; the contribution to energy related higher education is an important but secondary consideration. Thus projects sponsored at universities are essentially limited to advanced studies both theoretical and experimental usually performed by faculty members, staff research scientists, and doctoral candidates.

ENGINEERING RESEARCH PROGRAM
FY '83 BUDGET ($000's)
BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '83 BUDGET
BY TECHNICAL AREAS

	($000"s)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	1,739	33	32
SYSTEMS SCIENCES	2,061	37	17
ENGINEERING ANALYSIS	1,529	30	17

40-574 O - 85 - 30

AMES LABORATORY
Iowa State University
Ames, Iowa 50011

01. A COMPOSITE, MULTIVIEWING TRANSDUCER — $200,000 — 01-03, 81-3

James Corones, D. O. Thompson

The objective of this project is to demonstrate a composite, multiviewing ultrasonic transducer suitable for detecting, characterizing, and reconstructing flaws in structural materials for various applications. Development of this transducer utilizes a combination of recent advances in ultrasonic scattering and inversion theories with new concepts in transducer configurations and excitation methods. An experimental model of a composite transducer has been used as an aid in developing the semi-automated data acquisition and protocol. It has been determined that seven transducer elements which are multiplexed using both pulse-echo and pitch-catch modes are sufficient to produce good flaw reconstructions. Effects of limited aperture on the reconstruction have also been examined. The reconstruction protocol fits the acquired data to an "equivalent" ellipsoid of general shape (3 axes, 3 angles), a shape that is compatible with a fracture mechanics description of growing flaws and thus suitable for failure prediction. Criteria have also been established for individual transducer selection using experimentally determined scattering results. It is suggested that this procedure may form an approach for the further development of new transducer standards.

ARGONNE NATIONAL LABORATORY
Components Technology Division
Argonne, Illinois 60439

02. THEORETICAL/EXPERIMENTAL STUDY OF STABILITY CONTROL — $100,000 — 01-02 82-3

S. S. Chen, E. L. Reiss (Northwestern U), J. A. Jendrzjczyk

Theoretical and experimental studies are aimed at enhancing the understanding of nonlinear stability phenomena involving fluids, solids, and their coupling. The objective is to develop methods of controlling instability, and to explore the use of instability mechanics in engineering design. Studies of the mathematics of the modeled nonlinear systems are conducted at Northwestern University. Experiments and related analyses are performed at Argonne National Laboratory. The studies have been initiated with the special fluid-elastic stability problem of a slender elastic tube conveying fluid. In order to develop the required mathematical techniques and to understand the mathematical and physical phenomena that may occur, simpler oscillator problems are being studied in detail. These include the consideration of two simple, coupled nonlinear oscillators as a model to study secondary bifurcation of flutter. In parallel with the theoretical study, experiments are being performed with a tube, fixed at the upstream end and supported at a downstream location by a knife-edge support whose distance from the end can be varied. A series of exploratory tests has been performed and reported. Additional tests have focused on the region of transition from divergence to flutter and stabilization by means of external excitation at controlled frequencies, amplitudes, and location.

ARVIN/CALSPAN
Advanced Technology Center
P. O. Box 400
Buffalo, New York 14225

03. MITIGATION OF BIOFOULING USING SURFACE COATINGS — $ 0 — 01-02, 80-3

R. E. Baier, A. E. Meyer
R. W. King, M. S. Fornalik
H. Gucinski

Proceeding from calibration experiments in laboratory aquaria, two full-scale field trials have now been completed with special flow cells designed to assess the microfouling sequences and rates for diverse material/water compositions. Using thin, covalently bound organic films on test substrata allowing full analytical specification of fouling layer compositions, thicknesses, electrical, wetting, and textural features through time, it has been demonstrated that retention of both biofouling and scale-forming debris is minimized--without the need for toxic agents--when the critical surface tension is controlled at about 25 mN/m. It is particularly noteworthy that heat exchanger grade stainless steel, when modified with such thin surface-energy-control coatings, can be completely cleaned of fouling layers. Although the sequence of microfouling events observed has been common for all water types--saline, brackish, and fresh--tested so far, the fouling rates have been nearly ten-fold greater in the brackish waters on the Hudson River as compared with the fresh waters of the Niagara River.

BATTELLE-COLUMBUS LABORATORIES
Physical Metallurgy Section
505 King Avenue
Columbus, Ohio 43201

04. DAMAGE ACCUMULATION BY CRACK GROWTH UNDER COMBINED CREEP AND FATIGUE — $156,000 — 01-04 83-3

C. E. Jaske

The objective of this study is to develop and evaluate methods for assessing creep/fatigue crack growth under inelastic straining. A fracture-mechanics approach implementing the J integral for fatigue and the C* integral for creep is being employed. A computer program was developed for calculating creep/fatigue crack growth in laboratory specimens, and a crack-tip-zone interaction model was developed to account for the interactions between creep and fatigue during crack growth at high temperature. Experimental studies on Type 316 stainless steel at 593 and 649C are being continued, with emphasis on slow growth rates, and creep/fatigue crack growth studies of modified 9Cr-1Mo steel are being initiated. Three specimen configurations are being used: (1) low-cycle fatigue (LCF), (2) compact type (CT) and (3) center-cracked tension (CCT). The LCF specimens have short (0.05 to 1.5 mm) crack and the CT and CCT specimens have long (25 to 35 mm) crack. The range of the cyclic J integral is a good parameter for characterizing cyclic crack growth rates when creep effects are negligible. The C* integral is a good parameter for characterizing crack growth rates under static loading with steady-state creep across the remaining uncracked ligament. Transient fatigue-crack growth after a period of creep or transient creep-crack growth after a period of fatigue is being characterized and the results are being interpreted in terms of the crack-tip-zone interaction model. Future work will concentrate on examining the validity of this approach at slower fatigue- and creep-crack growth rates that are particularly relevant to many practical engineering applications.

BIPHASE ENERGY SYSTEMS
2800 Airport Avenue
Santa Monica, CA 90405

05. TWO-PHASE FLOW RESEARCH $0 01-02
D. M. Rovner 80-3

This is the concluding section of a three part program studying single and two-phase flow interactions encountered in the Biphase Rotary Separator Turbine. The objective is to experimentally determine the external drag exerted on a liquid flow pick-up penetrating the free surface of a liquid film, as occurs in the rotating separator of the Biphase turbine. The free surface of the associated wake downstream of the pick-up will also be determined. Drag, and free surface contour, is measured as a function on pick-up geometry, submerged length Reynolds number and submerged depth Froude number. Design recommendations to minimize external drag and related spray and wave generation will be made.

BROWN UNIVERSITY
Division of Engineering
Providence, Rhode Island 02912

06. IMPROVEMENT IN THE DESIGN AND EXTENSION OF OPERATING RANGE OF VISCOMETERS AND THERMAL CONDUCTIVITY CELLS
J. Kestin

$103,000 01-03 81-4

This project continues the development of measurement of two important transport properties, the viscosity and the thermal conductivity. Work is underway on the modification of existing instrumentation to extend the ranges of pressure and temperature and to make measurements at combined high temperatures and pressures (300-400 C and 30-40 MPa) while retaining the accuracy of 0.1-0.5% which is the state-of-the-art for more modest conditions. Working simultaneously in the same carefully staged way, the goal for thermal conductivity measurements is to develop instrumentation that will cover the range up to 50 MPa and 600°C. With each staged increase in capability, extensive measurements are being made on selected substances to secure results before the instruments are exposed to increased risk. New measurements on the viscosity of H_2O and D_2O were performed up to 200°C to create a basis for the search for a law of corresponding states. Preliminary calculations seem to point to the existence of such a law with appropriately chosen reference values. In the thermal conductivity instrument measurements on the mixtures of Ar-CH have been completed. The next step consists of a series of measurements on mixtures involving two gases of nearly identical molecular weight but different structure. Measurements on N_2-CO show that the mixtures have the same viscosity as N_2 or CO (both nearly equal), but significantly different thermal conductivity. This may prove of theoretical interest in statistical mechanics. The selected substances are chosen to make a contribution to the national energy program as well as to the development of methods of calculation for use in science and industry.

UNIVERSITY OF CALIFORNIA, LOS ANGELES
School of Engineering and Applied Science
Department of Mechanical, Aerospace and Nuclear Engineering
Los Angeles, California 90024

07. FLOW AND HEAT TRANSFER IN UNIFORM AND NON-UNIFORM POROUS BEDS — $61,000 — 01-02 83-4
Ivan Catton

The research covers two broad areas: 1) single-phase convection in porous media and 2) two-phase convection in porous media. The two areas of study are further sub-divided into a) forced convection, b) free convection, c) free/forced convection, d) fluidization under two-phase flow conditions and e) effects of bed non-uniformities. Layered porous media with intervening liquid regions as well as layers with no through flow will be part of the study. The objective of this research is to develop physical understanding of the governing phenomena and models for prediction of heat transfer by theoretical and experimental means. Previous work using the Glansdorff-Prigogine non-equilibrium thermo-hydrodynamic stability theory to address single-phase natural convection was extended to more realistically model the convective processes by including the additional quadratic inertial term suggested by Forchheimer in 1901. The momentum equation with the Brinkman extension to Darcy's law and the quadratic term allows us to study the effect of Prandtl number. A companion series of experiments are being carried out in a new apparatus. Experiments have been completed for steel and glass particle beds saturated with water. Results are in general agreement with earlier results. Measurements of wave number have also been made. Experiments are being run using silicon oil as the saturating fluid to yield a high Prandtl number. Future experiments will use mercury.

CALSPAN ADVANCED TECHNOLOGY CENTER
Aerodynamic Research Department
Buffalo, New York 14225

08. THE EFFECT OF AIR FLOW INSIDE A PNEUMATIC TIRE ON TEMPERATURE BUILDUP AND ROLLING RESISTANCE — $ 117,000 — 01-01 81-3

William J. Rae, George T. Skinner

The objective of this study is to quantify the effects of air flow and heat transfer inside a pneumatic tire on the temperature buildup and rolling resistance of the tire. The approach being followed has three phases: in the first, detailed measurements are being made of the flow velocities inside a tire under typical operating conditions. The principal experimental apparatus being used in these experiments is a set of hot-wire anemometers. In addition, pressures and temperatures will be measured at selected points. In the second phase, a computer program for predicting this flow will be developed, and its results compared with the experimental data. During the third phase, an energy-balance model will be developed, by means of which the flow and heat-transfer information developed in the first two phases will be translated into quantitative knowledge about energy losses due to the air flow. The overall result expected from this work is a method for assessing quantitatively the energy balance of the tire, as affected by load, road speed, inflation pressure, and other parameters.

UNIVERSITY OF CHICAGO
Enrico Fermi Institute
Chicago, Illinois 60637

09. FUNDAMENTAL AND TECHNIQUES OF NONIMAGING OPTICS FOR SOLAR ENERGY CONCENTRATION — $105,000 — 01-06 81-3

R. Winston, J. O'Gallagher

Nonimaging optics departs from the methods of traditional optical design to develop instead techniques for maximizing the collecting power of concentrating elements and systems. Designs which exceed the concentration attainable with focusing techniques by factors of four or more and approach the thermodynamic limit, are possible. This is accomplished by applying the concepts of Hamiltonian optics, phase space conservation, thermodynamic arguments and radiative transfer methods. Concentrators based on this approach are finding increasing use in solar energy and a variety of other applications and include the by now well known non-tracking Compound Parabolic Concentrator (CPC). To develop the underlying theory and design principles a theoretical formalism has been established based on a quantity called the geometric vector flux J, whose properties lead quickly to the discovery of new ideal concentrator solutions and an improved understanding of existing designs. Recently fundamental nonimaging optical principles have been extended to systems where physical optics effects play a role which has important consequences for concepts based on diffractive optics (e.g., holograms) and a promising method for deriving the vector flux yield for particular concentrator geometries based on the introduction of a pseudopotential, has been identified. Present objectives of this basic research program are to extend the development of these concepts not only for solar energy applications but for more general problems involving the transmission and detection of other portions of the electromagnetic spectrum as well.

CLARKSON COLLEGE OF TECHNOLOGY
Department of Chemical Engineering
Potsdam, New York 13676

10. BURSTING IN STEADY AND PULSATNG TURBULENT PIPE FLOW — $69,000 — 01-02, 82-3
J. B. McLaughlin and R. J. Nunge

The objectives of the research project are: (1) to gain an improved understanding of the production of turbulence in the viscous wall region of turbulent pipe flow; (2) to determine the effects of externally imposed pressure pulsations on turbulence structure and momentum, heat, and mass transfer in turbulent pipe flow; and (3) to determine the feasibility of exploiting such effects to increase the efficiency of heat exchangers and similar devices. A combination of computer modelling and laboratory experiments is being used to achieve these goals. The computer modelling involves the solution of a nonlinear, time-dependent model of the Navier-Stokes equation in which the axial and spanwise average of the axial component of velocity is set equal to a mixing length profile for all points lying outside the viscous wall region (which has a thickness roughly equal to 30 in wall variables) at each instant of time. In the case of steady turbulent flow, the model yields predictions for the intensities, production rate, and mean velocity profile which are in good agreement with experiment in the viscous wall region. In addition, detailed information about the structure and time dependence of the coherent eddies which dominate the production of turbulence in the viscous wall region has been obtained. The effect of pulsation on the behavior predicted by the model has been studied for a pulsation period equal to 100 in wall variables. It has been found that there is a large increase in the phase-dependent production of turbulence in the part of the cycle for which the bulk velocity is larger than average. Experiments are being carried out in order to check the predictions of the model about the effect of pulsations on momentum transfer and wall shear stress fluctuations.

COLORADO SCHOOL OF MINES
Department of Chemical and
Petroleum-Refining Engineering
Golden, Colorado 80401

11. RADIATIVE HEAT TRANSFER IN OIL SHALE RETORTING — $ 0 — 01-02, 81-2

Michael C. Jones

Successful modeling of oil shale retorting and other fossil fuel conversion processes depends upon an accurate knowledge of the transport processes occurring. Among these are the transport of heat between combustion gases and rock particles and the axial transport of heat along the retort. At the temperatures of the combustion zone in a retort, the dominant mode of heat transport between combustion gases and solids is radiation. The objective of this project is to provide a basis for modeling by experimental measurements and by evaluation of models of the heat transfer processes. The experimental method is to observe the propagation down a packed bed of inlet gas temperature disturbances, and to infer interphase heat transfer coefficients and axial conductivities by comparison with the results of a differential equation model containing those parameters. The comparison may be made in time, Laplace, or frequency domains. The effect of gas radiation will be determined by performing the experiment with carbon dioxide rich mixtures and with non-radiating gas (nitrogen or argon) as a control. Preliminary measurements on a two inch diameter bed led to the conclusion that heat loss at that diameter may predominate. Therefore a larger diameter bed with improved insulation is being constructed for this project. It aims at a temperature capability exceeding two thousand degrees Fahrenheit in order to guarantee the predominance of radiative transfer and to provide much needed high temperature interphase heat transfer data.

COLORADO SCHOOL OF MINES
Dept. of Chemical and Petroleum Refinig Engineering
Golden, CO 80401

12. MEASUREMENT AND CORRELATION OF HEAT TRANSPORT PROPERTIES FOR MODEL COAL LIQUID COMPOUNDS USING AN EXISTING HOT WIRE INSTRUMENT — $80,000 — 01-05 83-5

E. Dendy Sloan, Michael S. Graboski

The basic goal of this research is to determine some thermophysical properties of fluids encountered in the process of coal liquefaction. The research includes three major tasks. First, an expanded data base will be developed for coal liquids and model compounds. Second, these data will be tested against existing correlations for liquid thermal conductivity. Third, an instrument developed under a previous contract will be evaluated as a device for determining the thermal diffusivity of pertinent coal derived liquids.

CORNELL UNIVERSITY
College of Engineering
Ithaca, New York 14853

13. COMBUSTION CONTROL WITH SMART SENSORS — $115,000 — 01-03, 82-3
G. L. Wolga

The objective of this project is to develop a "smart" spectroscopic sensor suitable for monitoring gaseous combustion products by differential infrared absorption spectroscopy and to use the sensor to demonstrate closed loop combustion control of a two-burner furnace. The sensor is a computer controlled tunable acoustooptic infrared filter with sufficient resolution to resolve individual vibration-rotation absorption lines in the 5 - 6.5 micron spectral region. It will be self calibrating with respect to temperature changes and thus the sensor can operate unattended indefinitely. A tunable CO laser has been used to develop an accurate tuning curve for the filter in the 5 - 6.5 micron spectral region. Differential absorption measurements on CO and CO_2 in a heated cell are in progress to demonstrate the sensitivity of the filter, to select appropriate spectroscopic signatures, and to provide data for design of the self calibrating feature. Subsequently, infrared differential absorption spectroscopy will be carried out on combustion products from a flat flame burner; a turbulent, swirl burner; and finally, a two-burner furnance. This furnance will be fueled through control valves adjusted by a computer with the spectroscopic sensor providing quantitative information on combustion product concentrations sufficient to optimize furnance efficiency. Design and construction of the test burners is underway. Data analysis procedures for handling absorption integrated over a path length have been developed.

CORNELL UNIVERSITY
Department of Mechanical and Aerospace Engineering
Ithaca, New York 14853

14. FUNDAMENTAL HIGH PRESSURE DROPLET COMBUSTION CHARACTERISTICS OF EMULSIONS, MIXTURES, AND SLURRIES — $42,000 — 01-05 83-3

C. T. Avedisian

This work is designed to provide a fundamental understanding of the evaporation/combustion characteristics of unsupported droplets of emulsions, mixtures, and slurries in a high pressure gaseous environment. The affect of ambient pressure on both the droplet vaporization/burning rate and the intensity with which the test fuel droplets may undergo vapor expansions (i.e., microexplosions) during combustion will be studied. Several experimental and analytical efforts are planned. Droplet combustion experiments will be performed in a drop tower. In this technique, the combustion chamber, test droplet, and associated instrumentation are in free fall. Initial measurements planned include the effects of composition and ambient pressure on both the temporal variation of droplet diameter and vapor explosion intensity. This latter problem will also be studied in more detail in a second experiment designed to provide quantitative information on the specific mechanisms and parameters--pressure and liquid phase composition--controlling the vapor explosion of fuel droplets which are miscible mixtures of liquids. Light test droplets will be levitated and made to vapor explode in a flowing stream of another heavier immiscible field liquid in a vertical chamber, the pressure of which will be controlled up to 20 atm. Results will be compared to information relating to microexplosions obtained from the proposed drop tower experiments. Tasks completed and under development are the following: 1) a new and accurate method has been developed for predecting the liquid phase temperature required to initiate vapor explosions in multicomponent miscible liquids; 2) a model for bubble growth within superheated liquid droplets is under development; 3) the droplet levitation experiment is being constructed and 4) the drop tower is being designed.

ELECTROCHEMCAL TECHNOLOGY CORP.
3935 Leary Way, NW
Seattle, Washington 98107

15. ELECTROCHEMICAL WEAR MECHANISM AND DEPOSIT FORMATION IN LUBRICATED SYSTEMS — $69,000 — 01-01 82-3

T. R. Beck

The objective of this research is to measure and determine the importance of electrokinetic- or zeta- corrosion and deposit formation in lubricated rolling and sliding systems. Zeta corrosion is a phenomenon identified and modeled in 1968 for hydraulic servo control valves in commercial jet airplanes. This problem has now been solved by appropriate additives based on the theory. The approach of the present research is to compare measurements of wear for rolling and sliding lubricated systems to calculated zeta corrosion rates based on extensions of the valve wear model. The main challenge is distinguishing wear by zeta corrosion from abrasive and adhesive wear. In the first eight months of the contract required physical properties were measured for eight common lubricating oils and measurements were made of wall current density generated and size of wear scars. A good agreement was obtained between the measured wall current density and that predicted by the model for a simulated steel journal bearing. Wear on the plane polished journal turned out to be much greater than predicted by the measured and calculated wall current density based on the gross hydrodynamics. The wear scars consist of furrows with parallel scratches and furrows with micropits. With a Nylon cloth attached to the shaft wear scars are about the same size but virtually all pitted furrows. Zeta corrosion caused by passage of metal surface roughness or the roughness of the Nylon weave over the journal surface is indicated. Experiments to distinguish unambiguously zeta corrosion are underway.

GENERAL ATOMIC COMPANY
10955 John Jay Hopkins Drive
San Diego, California 92121

16. FLUID MECHANICS OF ACOUSTIC RESONANCE IN HEAT EXCHANGER TUBE BUNDLES — $ 95,000 — 01-02 82-3
R. D. Blevins

The purpose of this study is to develop a predictive fluid mechanic model for acoustic resonance in shell and tube heat exchangers. Acoustic resonance in heat exchangers is the result of acoustic oscillations of gas in sympathy with periodic fluctuations in the flow over tubes. In the experimental phase of the program, a simulated tube bundle is being constructed which will be tested in air flow. Direct measurements of the onset of resonance, intensity and mode of acoustic pressure will made with microphones, and measurements of the exciting fluid dynamic fluctuations about the tube will be made with hot wire anemometers. The results will be processed on-line using fast Fourier transforms. In the theoretical phase of the program, a linear acoustic model for the phenomenon will be developed using acoustic source and dissipation terms and a calculated acoustic mode shape. The experimental results will then be used to refine the acoustic source and dissipation terms, develop a fundamental understanding of the fluid dynamic and acoustic interaction. A nonlinear model for the self excitation will then be developed using Lighthill's formulation for aerodynamic sound in interaction with the coherent structures in the flow due to vortex shedding from the tubes.

GEO-CHEM RESEARCH ASSOCIATES
400 East Third Street
Bloomington, Indiana 47401

17. PREDICTIVE MODELING OF URANIUM ROLL TYPE DEPOSITS — $100,000 — 01-06 83-3
P. J. Ortoleva

Oxidizing meteoric waters percolating through a reduced sandstone aquifer can cause the accumulation of uranium and other ores at the redox interface. The oxidation of pyrite to hemtite or goethite can lead to several instabilities underlying observed ore body properties. The existence (and in some cases non-uniqueness) of propagating redox fronts in ore-reductant systems (such as pyrite) was demonstrated and a general exact value for its speed was obtained for the lossless aquifer. The nonexistence of constant velocity redox fronts in multireductant systems was proven analytically and shown numerically to correspond to an accumulation of one mineral at the front of the other - the essential trapping process leading to redox deposits.

A class of instabilities was found when reaction-induced porosity variations were allowed to interact with the percolation flow through the porosity-dependent permeability of Darcy's law. The planar front of dissolution of soluble components in a sandstone aquifer (as pyrite in oxidizing inflow waters) was found analytically to be unstable to the formation of bumps. The range of wavelengths of the most rapidly growing array of bumps brackets the observed wavelengths in roll front deposits when geologically reasonable flow and porosity values were used in our expressions. Numerical simulations of the full nonlinear problem confirmed the linear analysis, and showed that, interestingly, a single bump (in the shape of the surface on which porosity changes) can branch into two fingers. Even very small changes in porosity across the redox front can lead to this fingering.

Nonlinear transport/reaction interactions underly the genesis of uranium roll-front deposits and directly control their geometry and quality. These insights are potentially very useful for exploration.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Science Division
Idaho Falls, Idaho 84315

18. CRACK CHARACTERIZATION WITH ULTRASONIC NDE — $45,000 — 01-03 83-3

D. D. Keiser, J. A. Seydel
B. A. Barna, J. A. Johnson
D. M. Tow

The purpose of this research is to develop the instrumentation and analytical models that can predict and identify the frequency dependence of the amplitude and phase of ultrasonic echoes from defects. The approach treats the transducer/media/defect combination as a linear system which allows separation of the individual contributions to the signal detected at the transducer. A model based on the numerical solution of the partial differential wave equations has been developed to provide "snapshots" of the transducer field both before and after it has interacted with the flaw. This information is then compared to experimental data collected at a large number of transducer positions. Since the objective is to characterize defects, a number of techniques are being developed to display frequency-domain information which relates to the type of defect. One method is to display the phase and amplitude spectra values as a function of frequency and transducer position.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Technology Division
Idaho Falls, Idaho 83415

19.	ENGINEERING ANALYSIS OF ELASTIC-PLASTIC FRACTURE W. G. Reuter	$155,000	01-04 81-4

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluation guiding the direction of experimental testing. Tests are being conducted on a material (a modified ASTM A-710) exhibiting a range of fracture toughness but essentially constant yield and ultimate tensile strength. As test temperature increases, the specimen configuration-fracture toughness relationship complies initially with requirements for linear elastic-fracture mechanics and extends beyond the range of a J-controlled field. Presently, compact tension (3-point bend specimens will also be used in the future) are being used to develop state-of-the-art fracture mechanics data on the lower shelf (K_{Ic}), transition zone (J_{Ic}, J-R curves, etc.), and on the upper shelf (J_{Ic}, J-R curves, etc.). Results from the lower shelf and transition region are being used to predict failure conditions for specimens containing surface flaws. Predictions are then compared with experimental test data. These comparisons are presently underway for 6.4 and 12.7 mm thick surface-flawed specimens. Metallographic techniques are being used to measure crack tip opening displacement for comparison with analytical models. Laser interferometry and infrared thermography techniques will be used to evaluate and quantify the deformation in the crack region.

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
Department of Chemical Engineering
Urbana, Illinois 61801-3791

20. CONTINUOUS DAMAGE THEORY $39,000 01-04
Dusan Krajcinovic 83-3

The study centers on the phenomenological description of the nucleation and growth of microdefects in a metallic solid and their influence on the mechanical response. The analytical work will proceed within the scope of the Continuous Damage Mechanics, according to which the distribution and density of microdefects can be represented by a set of appropriately selected internal variables.

Present investigations focus on the basic aspects and definitions to prepare the groundwork and reconcile several different models. It was, for example, found that in case of a general microcrack field a distinction must be made between the microcrack distribution and the damage consistent representation of a field of flat microcracks. The projection of these vectors on a plane through the observed point is a physically reasonable measure of damage.

Subsequently the focus will shift on the investigation of the interaction of viscous effects (reflecting the boundary slip) and the brittle effects (growth of microcracks). The established continuum model will be used to study problems such as creep rupture, fatigue, etc.

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
Department of Chemical Engineering
Urbana, Illinois 61801-3791

21. CONDITIONS FOR DROPWISE CONDENSATION ON ELECTROPLATED GOLD — $ 0 — 01-02, 80-3
J. W. Westwater

This research is concerned with the use of thin coatings of gold, or possibly other noble metals, to produce dropwise condensation of steam on copper. Dropwise condensation is preferred to filmwise condensation, because it has much larger heat transfer coefficients. Numerous tests have been done with gold surfaces deposited by electroplating and by vacuum deposition. Analyses of the surface was by Auger spectroscopy and by electron microscopy. Success with gold has led to extension of the research to silver coatings. Distinct differences have been discovered. The minimum thickness of gold required for good dropwise condensation is 100 nm, whereas for silver it is 150 nm. A gold thickness of 200 nm will produce dropwise condensation for 12,000 hr. before deterioration of the surface is noted. With silver, a thickness of 300 nm begins to deteriorate in 200 hr., and a thickness of 3000 nm is required to achieve 1200 hr. To date the tests support a hypothesis that the role of the noble metal layer is to provide an oxide-free surface to which a trace of organic material can adhere firmly. The work is being directed to identify the source of the organic absorbent.

ILLINOIS INSTITUTE OF TECHNOLOGY
Department of Mechanical Engineering
Chicago, Illinois 60616

22. INTERACTIONS BETWEEN FRICTION-INDUCED VIBRATION AND WEAR — $80,000 — 01-02 82-2

V. Aronov, A. F. D'Souza
S. Kalpakjian

The objective of this project is to gain knowledge of the influence of system stiffness and vibrations on friction and wear. There is increasing evidence, both from our previous studies and from the very limited literature available, that in addition to the role of various physical, chemical and mechanical parameters, the dynamic characteristics of the equipment or machinery involved also have a significant influence on friction and wear. This project involves an interdisciplinary study to investigate the interactions between friction-induced vibration and wear. The major experimental parameters are the normal, tangential and torsional rigidity in a sliding system and different lubricating conditions, with observations and analysis of wear surfaces and particles. Among the subjects being studied are the effects of system stiffness and load on the different regimes of friction, vibrations, and wear. A mild wear model has been developed to account for effect of system stiffness. The transition from mild to severe wear is being investigated. A stability theory is being developed to explain the onset of friction induced self-excited vibrations. Physical and mathematical models of oscillations are also being developed, including the effects of surface alterations due to wear.

ILLINOIS INSTITUTE OF TECHNOLOGY
Department of Electrical Engineering
Chicago, Illinois 60616

23. METHOD OF VIBRATIONAL CONTROL IN THE PROBLEM OF STABILIZATION OF CHEMICAL REACTORS — $ 0 — 01-03, 80-3

S. M. Meerkov

The objective of this research is to develop the vibrational control technique for complex nonlinear dynamic systems with multiple steady states and limit cycles. From the mathematical standpoint, the goal of the project is to analyze the effects of fast parametric oscillations on the system's dynamics. During the third year of the project, the conditions of vibrational stabilizability of nonlinear systems were investigated. It was shown that in the case of linear multiplicative vibrations the conditions of vibrational stabilizability depend on the linear part of the system; in the case of periodic forcing, on nonlinear part of the system, and in the case of vector additive vibrations, on both. The developed approach was applied to analysis on autocatalytic (Van de Vusse - type) reaction in a CSTR with oscillating input flow. It was shown that, unlike exothermic and catalytic reactions where the increase in productivity is achieved due to the straightening of the negative slope of the steady state characteristic, in the autocatalytic case the increase in productivity is ensured by an additional, input-like term. The results of numerical investigations supported this analytical finding.

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, CA 91109

24. BASIC DATA FOR THE DEVELOPMENT OF MOLECULES AS THRESHOLD ELECTRON DETECTORS — $65,000 — 01-03 82-3

A. Chutjian, S. Alajajian
J. M. Ajello

Measurements and calculations are being made of, at high electron energy resolution, lineshapes and cross sections for attachment of thermal electrons to a number of electron-attaching gases. Perfluorinated carbon and chlorofluorocarbon compounds have been shown to be viable candidates for use a molecular detectors for extremely low-energy (0-50 millielectron volt) electrons. The use of such detectors has been demonstrated in our own laboratory in obtaining the first threshold photoelectron spectra of N_2, CO and O_2 by the TPSA technique. Both SF_6 and $CFC\ell_3$ were used as detectors. It is desired to study the use of other gases, as well as temperature effects, to obtain the narrowest bandwidth for zero-energy electron detection. It is also desired to explore the s-wave nature of the attachment onset which gives rise to a divergent, hence harrow, cross section in the limit of zero electron energy. Preliminary results have been obtained for the gases $CC\ell_4$ and $2\text{-}C_4F_6$. Clear indications for the s-wave divergence of the dissociative attachment cross section in $CFC\ell_3$ have been obtained. These molecular detectors have applications in threshold photoelectron spectroscopy, in the design of high-power switches, and in the refinement of tracer gas techniques for studying rates and directions of air motion. Theoretical calculations in a local quantum formulation are carried out in parallel to correlate cross sections and attachment widths with the potential energy surfaces of the ground neutral and negative-ion states.

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, CA 91109

25. THIN FILM CHEMICAL SENSORS BASED ON ELECTRON TUNNELING — $120,000 — 01-03, 82-3
J. Lambe, S. K. Khanna

The objective of this three year program is to understand the physical mechanism of detection underlying a totally new chemical detection concept which utilizes electron tunneling as the sensing mechanism. The technical approach involves investigations of the tunneling spectrum (second derivative of current with respect to voltage versus voltage) of metal oxide-metal (e.g., aluminum-aluminum oxide-gold) tunnel junctions which are exposed to chemicals such as halogens. Some of the other key questions to be addressed in this project are: 1) what are the ultimate sensitivity and selectivity, and 2) what are the contributions of the insulating layer and the top porous metal electrode. These electrical measurements, in addition to surface and interface studies, should help us to understand the detection mechanism. A successful program can pave the way for the development of a compact thin film electronic chemical sensor for use in the automation of the chemical processes, and hence, to increase reliability and productivity. Al-Al_2O_3-Au (MIM) tunnel junctions were fabricated using an oil-free ultra-high vacuum system. The iodine signal was observed by measuring the tunneling spectrum of the MIM tunnel junction exposed to iodine vapors. We have also observed the intrinsic surface state on gold surface using electron tunneling spectroscopy. These surface states have been identified as playing a key role in the chemical detection mechanism.

LAWRENCE BERKELEY LABORATORY
Physics Division and
Accelerator and Fusion Division
University of California
Berkeley, California 94720

26. STUDIES IN NONLINEAR DYNAMICS $ 90,000 01-06
Allan N. Kaufman, Henry D. I. Abarbanel 80-3

This project involves studies of fundamental properties of non linear dynamical systems which arise in physical situations of importance to energy research. Three main subjects are being explored. First, theoretical studies to generalize the WKB representation of wave phenomena are in progress. In this work, caustics are avoided by working in a space of enlarged dimensionality. Propagation of short wave length signals is then treated in a regular, non-linear fashion in phase space. Second, the transport properties of conservative and dissipative non-linear systems described by systems of ordinary differential equations are investigated. Transport equations have been derived and the transport coefficients expressed as integrals over correlation functions of state space. Transport properties of fluids which allow a reasonable mode truncation (Galerkin approximation) are given by these methods. Current work is focused on evaluating the asymptotic attractors and computing physically important correlation functions on the attractor. Third, investigations of analytic techniques for determining the position in parameter space and nature of bifurcations from periodic orbits are underway. Analytic methods based on center manifold theory and Poincare normal forms are being developed to study the stability of limit cycles which arise in a Hopf bifurcation from steady orbits. Applications to fluid flow and oscillations in non-linear phenomena of importance to energy systems are the testing grounds for the mathematical techniques.

LAWRENCE BERKELEY LABORATORY
Energy and Environment Division
University of California
Berkeley, California 94720

27. CONTROLLED COMBUSTION — $160,000 — 01-05
A. K. Oppenheim — 79-6

The principal objective of this study is the acquisition of fundamental knowledge required for the development of controlled combustion systems. Such systems offer the prospect of maximizing thermal energy conversion efficiency, minimizing pollutant emissions, and optimizing the tolerance to a wide variety of fuels. A thorough understanding of ignition--the initiation of a self-sustained exothermic process of combustion--is for this purpose of essential importance. The major objective of the experimental program is the establishment of the required background for the design of enhanced ignition systems. Of prime importance in this respect is the determination of the role of active radicals. This is accomplished by the use of a high frequency response molecular beam mass spectrometer that has been designed and built especially for this purpose. The corresponding theoretical approach is based on an extended thermo-chemical analysis as set forth by Semenov and Frank-Kamenetskii for auto-ignition in a closed system. This is supplemented by numerical modeling of jets and flame propagation in turbulent flow. The experimental testing program is in progress with flash photolysis of NO_x used to ignite a helium diluted hydrogen-oxygen mixture. In the concomitant analytical studies we have been able to deduce the classical first, second and third auto-ignition limits from a self-consistent theory, and to model the formation and inflammation of a turbulent jet.

LAWRENCE LIVERMORE NATIONAL LABORATORY
Engineering Division
P. O. Box 808
Livermore, CA 94550

28. PROCESSING AND CHARACTERIZATION OF SCATTERED SIGNALS FROM ACOUSTIC TARGETS — $100,000 — 01-03 82-4
B. Maxfield, E. Miller

We have begun in FY 1982 a study to develop a fundamental understanding of acoustic scattering from targets having relevance to material strength, for example flaws in metal components and welding faults, and to process such target signatures for possible automatic material characterization in nondestructive evaluation (NDE). This work is related to instrumentation development for NDE and more specifically with electromagnetic/acoustic scattering, and signal processing research. LLNL is currently involved in both areas using internal funds (engineering research) as well as reimbursable support (from various DOD agencies, and NRC).

LOS ALAMOS NATIONAL LABORATORY
Electronics Division
Los Alamos, New Mexico 87545

29. DEVELOPMENT OF INTEGRATED THERMIONIC CIRCUITS — $160,000 — 01-03 82-3

B. McCormick, D. Wilde, D. Lynn, R. Dooley

The object of this project is to develop electronics that are capable of operating in both high-temperature and high-radiation environments while maintaining levels of circuit sophistication, integration, and reliability demanded of modern electronics. The approach taken for these active electronic gain devices has been to use the intrinsically high-temperature phenomenon of thermionic emission in conjunction with the thin-film technology of integrated circuits to produce microminiature vacuum triodes. High-temperature tests have been conducted at 500 C for approximately 13,000 hours with no degradation in device characteristics. Devices have been subjected to total radiation doses of 10 neutrons/cm and 2.5 x 10 rad and radiation pulses of 1.4 x 10 neutrons/cm /s and 1.2 x 10 rad/s with damage. More complete tests of transient gamma effects will be completed during the upcoming fiscal year, at which time, integrated flip flops (memory cells) will be tested. It was determined that the source of resistive leakage between elements was due to the reduction and deposition of hydrocarbons present in the photoresist used to define the cathode pattern. The cathode development process and the cathode coating have been changed to reduce the hydrocarbons present resulting in a leakage reduction (two orders of magnitude) to a level acceptable for circuit development.

UNIVERSITY OF MARYLAND
Department of Mechanical Engineering
College Park, Maryland 20742

30. NUMERICAL MODELING OF TURBULENT ENERGY RELATED FLOWS — $ 18,000 — 01-02, 81-3

B. S. Berger, P. S. Bernard

The objective of this research effort is computational modeling of turbulent energy related fluid flows with a view to the calculation of the lift and drag forces acting on the individual tubes of a heat exchanger tube bank. The MVC turbulence closure has served as the basis for the computation. Results derived from the previous year's research have appeared in four journal publications. The first two pertain to the derivation of the closure field equations in 3-D and their specialization to cylindrical geometries. The second two are studies of dissipation in the boundary layer involving microscales, correlation tensors and the balance of turbulent energy in the linear wall region. Current efforts have concentrated on the numerical aspects of the application of the MVC closure to cross flows over circular cylinders. In this regard the computation of velocity correlations from vorticity correlations is of particular importance and has led to successful theoretical and computational studies of the symmetry of correlation functions, the numerical integration of Green's functions and the computation of velocity fluctuations from vorticity fluctuations. These results have been incorporated in a computer code which is undergoing numerical verification for the crossflow problem.

UNIVERSITY OF MASSACHUSETTS
Chemical Engineering Department
Goessmann Laboratory
Amherst, Massachusetts 01003

31. SHORT-CUT PROCEDURES FOR THE SIMULTANEOUS DESIGN OF A PROCESS AND ITS CONTROL SYSTEMS — $0 — 01-03, 81-3

J. M. Douglas, M. F. Malone

Cost models based on short-cut designs for whole plants have been completed, and used to estimate the optimum process design conditions. This is necessary to evaluate the impact of disturbances and the effect of control. The major process interactions and alternatives included so far are: the effect of operating pressure level in distillation on reboiler and condenser heat loads, the influence of reactor conversion on the distillation sequence, and the heat exchange network for the whole process. Simplified models for the design, optimization and steady-state control of several alternative distillation configurations have been developed. Significant changes in the overall process economics as well as coupling of the optimal configuration, recycle purity and reactor conversion are found. Further synthesis studies, particularly for the case of sidestream and configurations of sidestream columns, are continuing.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, Massachusetts 02139

32. TURBULENT PREMIXED FLAME STUDY — $130,000 — 01-05 83-3
Wai Cheng, James Keck
Steve Pope (Cornell University)

This program is a combined experimental and theoretical study of premixed turbulent flames. The primary aim of the experiment is to study the gross behavior and some detailed properties of statistically spherical flames over a very wide range of operating conditions. It is emphasized that the range of operating conditions is sufficiently wide to encompass qualitatively different regimes of combustion. The theoretical part of the program centers on calculations of the joint probability density function (pdf) of the velocity and species concentrations. This approach - to solve a transport equation of the joint pdf - avoids the closure problem normally associated with turbulent velocity fluctuations and non-linear reaction rates. In both the experimental and the theoretical effort, the primary variables being examined, for a flame of a given geometry and fuel/air ratio, are a Reynolds number based on the turbulent strain rate, and a Damkohler number based on the ratio of the eddy time to the chemical reaction time. A premixed flame combustion wind tunnel has been constructed. The facility can be operated both in the continuous flow and in the blow-down mode. In the latter mode, a vacuum dump tank is incorporated to create a sub-atmospheric test section pressure for wider range of test conditions. In the theoretical study, preliminary calculations relating the normalized flame speed to the Damkohler number using the pdf formulation has been attempted. A "variable weighted" algorithm to treat the density difference between the burned and unburned mixture is being developed.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Laboratory for Manufacturing and Productivity
Cambridge, Massachusetts 02139

33. A STUDY OF REDUCED ORDER MODEL REFERENCE CONTROL SYSTEMS FOR IMPROVED PROCESS CONTROL — $ 49,000 — 01-03 82-3

David E. Hardt

The objective of this research is to provide a method for easy design of control systems when the plant involved is highly variable in both structure and parameter values. This typifies many manufacturing processes, which in general are highly sensitive to intrinsic properties of the infeed material, have poorly understood or controlled boundary conditions, and often have highly non-linear characteristics. In addition, the disturbances most frequent in a manufacturing process are best characterized as parameter changes rather than state variable changes. The choice of a parameter adaptive control paradigm is obvious since it has the property of optimizing system response characteristics in the face of wide plant parameter variations. Model Reference Adaptive Systems enjoy an ease of design and performance specification, and again seem applicable; however, there is a restriction within current theory that the plant be characterized in its structure well enough to have a reference model of identical order. This restriction implies a static plant structure and more a priori knowledge than is often present. In this research the implication of a reduced order (or mis-matched) reference model is being investigated.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, Massachusetts 02139

34. PISTON RING FRICTION AND VEHICLE FUEL ECONOMY — $35,000 — 01-01, 80-3
D. P. Hoult, J. M. Rife

The purpose of this research is to study the friction mechanism in automotive engines, in particular the components of frictional losses which arises due to the interaction between the piston rings and the piston liner. It is believed that this is the largest single component of friction in a typical automotive engine. The research underway comprises modelling and measuring the motion of each degree of freedom model of piston ring as it moves up and down in the piston groove has been completed and modifications necessary for the theory have been described. The next steps of this project, which are underway, are to study the ring twist and radial motion of rings in a experimental lubrication engine. The theory has suggested a novel concept for a gas lubricated ring which may greatly reduce engine friction.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Laboratory for Manufacturing and Productivity
Cambridge, Massachusettts 02139

35. IMPROVEMENT OF RELIABILITY OF WELDING BY IN-PROCESS SENSING AND CONTROL — $100,000 — 01-03 79-6

Koichi Masubuchi, Henry M. Paynter,
David E. Hardt, William C. Unkel

Over the years, the cost of constructing critical welded structures has increased drastically. A significant portion of the increase comes from required inspection and repair, while the direct cost of welding has increased only slightly. Closed-loop control of the welding variables represents a promising cost-effective approach to improving weld quality and therefore reducing the total cost of producing welded structures.

This research program includes the following tasks:

(1) Demonstration of the measurement of weld size using mechanical impedance as a sensing technique for one of the two weld geometry measurements,
(2) Demonstration of a single variable control system using the above measurement,
(3) Demonstration of the ability to gain independent control of two weld geometry measures as described, for example, by the front and back bead widths of the weld metal,
(4) Demonstration of closed-loop geometry control with these two control variables,
(5) Expand the variables to be controlled from two geometry measures to include temperature history of the weldment,
(6) Implement the geometry control system on a mechanized welding system, and
(7) Provide one formal framework for implementation of welding control.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Nuclear Engineering
Cambridge, Massachusetts 02139

36. HYDRODYNAMIC PREDICTION OF MULTIDIMENSIONAL SINGLE- AND TWO-PHASE FLOW IN ROD ARRAY — $60,000 — 01-02, 82-3

N. E. Todreas
J. T. Robinson

The objective of this research is to develop basic constitutive laws for the hydrodynamics of flow oblique to rod arrays. A thorough knowledge of the flow field within heat exchanging components comprised of rod arrays (i.e., heat exchangers, steam generators, nuclear reactor cores, condensers) is of primary importance to maintaining a high component efficiency, lifetime, and operational performance. Much thermal-hydraulic design and operational performance analysis of these energy components is being performed with discretized computer models. The recent advancements in high-speed digital computers and numerical computational methods have facilitated the expansion of these thermal-hydraulic codes from one- to two- and three-dimensional multiphase flow analysis. These new codes require as input constitutive laws of multidimensional, single- and two-phase flow fields within rod arrays such as those being developed in this project. Specifically, constitutive relations for single-phase flow resistance, two-phase flow resistance, and relative phasic motion (slip) will be developed based on measurements using atmospheric air/water within vertical test sections comprised of rod arrays inclined at 0, 30, 45, and 90 degrees to the direction of flow. Major tasks completed to date include (1) an evaluation of multidimensional flow resistance models for single phase turbulent flow, and (2) formulation of a model for relative phasic motion for bubbly flows.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, Minnesota 55455

37. FLOW AND HEAT TRANSFER WITH IMPINGING JETS AND WALL JETS — $ 88,000 — 01-02, 81-3
R. J. Goldstein

This project is planned to provide information on flow of impinging jets and wall jets. Measurements of the heat transfer in the region of impingement will be obtained for single jets entering a still ambient, for jets entering a crossflow, and for various two-dimensional arrays of jets. In addition to quantitative heat transfer measurements for these flows, visualization techniques will be used to provide insight into the mechanism of the interaction of the jets and the local wall shear. A laser-Doppler anemometer is being developed to provide detailed measurements of velocity distributions, velocity fluctuations, and Reynolds stresses in a plane wall jet. Design of this system is complete and construction is nearing completion. Such measurements should provide precision data for testing the validity of turbulent transport models that have been suggested. To date, significant data have been obtained with a single jet; the results of several series of tests have been correlated with equations for both the peak heat transfer coefficient and the average heat transfer coefficient over various regions from the center of impingement. Also, some data have been taken for a two-dimensional array of small jets impinging on a heat transfer surface. During these latter studies, a liquid crystal system was developed for studying the features of single and multiple jet rows on a flat surface. Development of the liquid crystal technique and study of the pressure distribution near individual jets on an impinging jet plate is a new element introduced into the project as the effort got underway. It should add significantly to the initially planned scope of the project.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, Minnesota 55455

38. FUNDAMENTAL HEAT TRANSFER PROCESSES RELATED TO PHASE-CHANGE THERMAL STORAGE MEDIA — $63,000 — 01-02 80-3

E. M. Sparrow

This research program deals with the fundamental heat transfer processes which occur in phase-change thermal storage systems. The present focus of the work is on phase change which occurs within a closed cylinder or tube. In separate but interrelated freezing and melting experiments, the effects of the inclination of the tube in the gravity field are being investigated. For freezing, despite local variations, the global (i.e., surface-averaged) freezing rate is virtually independent of the inclination of the tube. On the other hand, for melting, different regimes characterized by different melting rates occur as a function of the tube inclination. The rate of melting is least when the tube is vertical. At moderate angles relative to the vertical, gravity presses the melting solid against the tube, thereby accelerating the rate at which melting occurs. The acceleration of melting due to inclination is being explored as a means for recouping reductions in melting rate which occur when the containment tube is nonuniformly heated, as is the case when the tube is heated by solar energy. In another set of experiments, freezing in a rotating tube is being investigated.

NATIONAL BUREAU OF STANDARDS
Thermophysics Division
Washington, D.C. 20234

39. THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES — $300,000 — 01-03 82-2
H. J. Raveche, N. Olien

This project aims at the development of accurate measurement capabilities for the thermophysical properties of complex, multi-phase, fluid mixtures containing hydrocarbons. The research is being done jointly by the Thermophysical Properties Division, at the NBS-Boulder facility and the Thermophysics Division at NBS-Gaithersburg, both within the NBS Center for Chemical Engineering. The properties involved are PVT (pressure-volume-temperature), phase equilibria (liquid-vapor and liquid-liquid equilibria) and transport properties (viscosity and thermal conductivity). The apparatus will be designed for use in corrosive, highly corrosive, and sometimes toxic and flammable fluids with measurements extending to high temperatures (900 K) and high pressures (30 MPa and in some cases 70 MPa). Current work involves: 1) construction of a constant-flow phase equilibria apparatus covering the range 300-800 K with pressures to 30 MPa or more; 2) construction of a multicomponent-multiphase nonsampling cell for temperatures to 470 K and pressures to 10 MPa; 3) design and construction of new phase equilibria apparatus to cover the range 250-350 K with pressures to 20 MPa; 4) automation of an existing Burnett PVT apparatus for the range 270-470K; 5) construction of a magnetic balance densimeter for the range 270-470 K with pressures to MPa; 6) design of a torsional crystal viscometer for the range 300-750 K with pressures to 50 MPa or more; and 7) initiate design of high temperature thermal conductivity apparatus. Future work will include completion of the apparatus, performance testing, and the start of measurements on systems relating to long-term energy needs, such as polar-nonpolar mixtures found in the reaction products of the conversion of solid fuels to liquid and gaseous fuels and chemical feedstocks. In addition, other measurement techniques will be explored such as acoustic properties, light scattering, etc.

NATIONAL BUREAU OF STANDARDS
Office of Standard Reference Data
Washington, D.C.

40.	SUPPORT OF CRITICAL DATA COMPILATIONS David R. Lide, Jr.	$450,000	01-05 80-6

The Office of Standard Reference Data administers a collaborative interagency program for preparation of compilations of physical and chemical reference data. Each project supported is expected to lead to a publishable data compilation containing recommended values and accuracy estimates for the data set in question. Projects funded during fiscal year 1983 include work on high temperature vaporization of metal oxides; electrochemical equilibrium data on iron-water systems; thermodynamic properties of vanadium-niobium alloys; refractive indices of optical materials; properties of aqueous electrolytes at high temperatures; atomic transition probabilities of highly ionized atoms; thermodynamic tables for hydrocarbon isomer groups; ESCA data; solubility of polyaromatic hydrocarbons and of zinc, cadmium, and copper salts; ceramics phase diagrams; and alloy phase diagrams for systems of iron, alkali metals, and rare earths.

This project is included in the BES ENGINEERING RESEARCH program for administrative convenience. Coordination with NBS is accomplished in collaboration with the BES Chemical Sciences and Materials Sciences divisions. BES FY 1982 funds for the project were provided by the Chemical Sciences and Materials Sciences divisions.

CITY UNIVERSITY OF NEW YORK
The City College
Department of Chemical Engineering
New York, New York 10031

41. TOPICS IN PHYSICO-CHEMICAL HYDRODYNAMICS — $260,000 — 01-06, 80-8
Benjamin G. Levich

This research comprises two main directions:

(i) Fully Developed Turbulence (FDT). We aim at the entirely novel understanding of the nature of FDT. We assert that the structure of FDT is determined by a foam-like topology of the vorticity field lines where the prime role is played by the hierarchy of helical fluctuations. The active production of turbulence in this picture proceeds outside of these fluctuations and concentrates in space of fractal dimensionality. Presently, we have a rather extensive experimental data to support our view. Further experiments are underway.

(ii) Interfacial Mechanics.

(a) A mechanism for the development of the deformation patterns commonly observed on the surfaces of biological cell plasma membranes was suggested. In this mechanism, the membrane is treated as a viscoelastic continuum and a chemical reaction network on the surface of the membrane regulates the membrane elasticity.

(b) Hydrodynamic waves induced by chemical reactivity waves was studied. Results indicate that a wave of chemical reactivity derived from a multistable chemical reaction on the surface of a thin liquid film is able to induce a hydrodynamic wave in the film through the Maragoni tractions due to the reactivity wave.

(c) The classical linear capillary instability of a thin fluid filament surrounded by a bulk fluid was investigated for the case in which the filament is in steady shear flow. Results indicate that a nonlinear interaction between the shear flow and the capillary forces can, under certain conditions, stabilize the developing linear instability.

NORTHWESTERN UNIVERSITY
Chemical Engineering Department
Evanston, Illinois 60201

42. CONVECTIVE BOILING HEAT TRANSFER IN NARROW ANNULAR GAPS — $ 0 — 01-02, 81-3

S. G. Bankoff, R. S. Tankin, M. C. Yuen

Commercial nuclear steam generators are subject to accelerated stress-corrosion due to thermal cycling in the crevices between the boiler tubes and tubesheets, probably resulting from periodic rewetting and dryout. The objective of this research is to study boiling heat transfer in these short narrow gaps, using a two-loop system, with a primary water side operating at 17 bars, and the secondary steam-water side up to 7 bars. Heat transfer coefficients over the full range of conditions, from subcooled nuclear boiling to dispersed droplet-flow conditions, will be measured. Improved correlations, taking into account the crevice L/D effect, will be thus obtained. A theoretical analysis of the periodic dryout and rewet phenomenon is also planned.

NORTHWESTERN UNIVERSITY
Department of Civil Engineering
Evanston, Illinois 60201

43. EFFECTS OF CRACK GEOMETRY AND NEAR-CRACK MATERIAL BEHAVIOR ON SCATTERING OF ULTRASONIC WAVES FOR QNDE APPLICATIONS — $53,000 — 01-03 83-3

J. D. Achenbach

Among the methods of quantitative non-destructive evaluation of structural elements, the method based on scattering of ultrasonic (elastic) waves by flaws is particularly useful. The work on this project is concerned with applications of the scattered field approach to the detection of a cracklike flaw, and to the determination of its location, size, shape and orientation. Interior, as well as surface-breaking and near-surface cracks are considered. The usual mathematical modeling of ultrasonic wave scattering by cracks is adjusted to account for several typical characteristics of fatigue and stress-corrosions cracks, and the environment of such cracks. Effects due to crack-face roughness, crack-closure and crack-face interactions are considered, as well as global anisotropy. Local anisotropy and inhomogeneity due to near-tip voids, and the effect of a zone of plastic deformation near a crack tip will also be investigated. Parametrical studies are expected to display the masking of characteristic "crack-like" features of the scattered field by a spectrum of signals due to deviations from an idealized crack geometry and idealized material behavior. Progress has been made on the effects of crack-face interactions and global anisotropy.

PACIFIC NORTHWEST LABORATORY
Engineering Physics Department
Richland, Washington 99352

44. HOLOGRAPHIC INVESTIGATION OF THERMAL-NONEQUILIBRIUM VAPOR GENERATION IN TWO-PHASE FLOWS — $125,000 — 01-02 81-3

J. M. Creer, J. M. Bates, B. B. Brenden, J. L. Daniel

The principal objective of the research is to gain a basic understanding of the thermal nonequilibium vapor generation process. Nonequilibrium vapor generation is known to have major implications in the analysis of postulated Loss of Coolant Accidents (LOCA) for light water nuclear reactors as well as being important to the analysis and development of alternate energy sources such as geothermal, liquified natural gas, and solar. Single and double pulse holographic optical recording techniques and associated image analysis capabilities are being utilized to permit detailed three-dimensional characterization of two-phase flow fields in regions of thermodynamic nonequilibrium. Two-phase flow fields will be formed in rapidly depressurizing, recirculating flow through a specially designed convergent-divergent nozzle assembly. The first two years of the proposed three-year project have been devoted to optimizing holocamera systems, developing appropriate software for a semiautomated contrast scanner/image analysis system, and designing and procuring hardware for FY 1983 tests in a closed loop high pressure/temperature thermal hydraulic facility. Data acquisition and reduction will be completed in FY 1984.

UNIVERSITY OF PENNSYLVANIA
Department of Mechanical Engineering
and Applied Mechanics
Philadelphia, Pennsylvania 19104

45. CRACK-TIP FIELDS FOR MATERIALS WITH EXPONENTIAL-LAW-CREEP BEHAVIOR AT HIGH STRESS — $136,000 — 01-04, 83-4
John L. Bassani

This research is concerned with elastic-viscoplastic analyses of cracks under creep conditions, with particular emphasis on the influence of the assumed stress dependence on the creep strain-rate. At high stress levels the creep strain-rate for many (if not most) structural materials varies as the exponential of stress while at low stress levels it varies as stress to some power. The complete stress dependence is given by the hyperbolic-sine-creep law $\dot{\varepsilon} = \dot{\varepsilon}_0 [\sinh(\sigma/\sigma_0)]^n$. Based on this creep law an asymptotic analysis demonstrates that the notch-tip stress intensification is weaker and the strain-rate intensification is stronger than for a power-law material. Under extensive creep conditions the path-independent integral C^* is the relevant fracture parameter. In small-scale-yielding at relatively low applied load levels the elastic stress intensity factor K_I is the relevant parameter; the high load case is being investigated numerically. Finite element calculations show that in small-scale yielding relaxation around the crack-tip follows $\sigma\dot{\varepsilon} \propto 1/t$ as in the power-law case. Current work includes finite element calculations and modeling of the crack growth process by grain-boundary cavitation in the hyperbolic-sine crack-tip fields.

UNIVERSITY OF PENNSYLVANIA
Department of Electrical
Engineering and Science
Philadelphia, PA 19104

46. HIGH TEMPERATURE CHEMICALLY SENSITIVE ELECTRONIC DEVICES — $100,000 — 01-03 82-3

J. N. Zemel, I. R. Lauks,
S. Yuen, J. Wei

Monitoring the chemical environment in an aqueous saline solution is a major problem in geothermal environments. Additionally, the kinetic behavior of aqueous solutions in the temperature range from 0-250° C and pressures from 0-5000 psi have not been fully investigated. The purpose of this program is to develop the scientific and technological knowledge which will permit real time analysis of the chemical behavior of aqueous saline solutions in this temperature and pressure regime. The approach adopted has been to develop a chemically sensitive electronic device based on a specially designed and constructed gate controlled diode (ICD). These devices have been demonstrated to operate up to 200°C. IrO reactively sputtered films have been shown to survive 200°C at 4000 psi in distilled water for periods in excess of four hours without any observable degradation. In the past six months, a four element (ion) structure has been designed and preliminary data obtained on its operation. Continuing measurements on IrO stared in water for a year showed that the layers would survive with a pH response that was reproducible to better than 10mV. Continued efforts are planned on characterizing the IrO layers and completing the four element sensor.

RICE UNIVERSITY
Department of Chemical Engineering
Houston, Texas 77251

47. MEASUREMENT AND PREDICTION OF LIQUID MIXTURE THERMAL CONDUCTIVITY AND VISCOSITY — $40,000 — 01-05 82-3

R. L. Rowley

In spite of the importance of liquid mixture thermal conductivities and viscosities in energy technology, existing models and correlations are either inaccurate and inadequate or require multiple adjustable parameters for each specific system. This project has led to the development of a new predictive method for liquid mixture thermal conductivities and shear viscosities, based on the local composition concept for nonrandom liquid mixtures, which permits accurate estimation of these properties from thermodynamic data with no adjustable parameters. A high-precision capillary viscometer has been used to study a wide range of binary and ternary viscosities over a moderately wide temperature range at ambient pressure. These data have been used to test the newly developed model. Although the model contains only binary interaction terms obtained from equilibrium thermodynamic information, ternary as well as binary systems are accurately predicted by this method. Test system emphasis has been on highly nonideal mixtures containing polar and associating components. The temperature dependence of these mixture viscosities and the nature of aqueous systems are currently under investigation. Additionally, a new transient hot-wire thermal conductivity cell capable of making rapid and accurate liquid mixture thermal conductivity measurements has been designed. Construction of the apparatus is in progress. The local composition model has been used to make both binary and ternary mixture thermal conductivity predictions; while the binary results have been extremely accurate when compared to literature data, hardly any ternary mixture data have been found with which to compare the predictions. Experimental data obtained during the next year from the new thermal conductivity cell should remedy this situation.

ROCKEFELLER UNIVERSITY
Department of Physics and Mathematics
1230 York Avenue
New York, New York 10021

48. SOME BASIC RESEARCH PROBLEMS RELATED TO ENERGY — $ 0 — 01-06, 81-3
Kenneth M. Case, E.G.D. Cohen,

This project is concerned with investigations of three specific areas: 1) The prediction and evaluation of thermophysical data of fluids and fluid mixtures, 2) The statistical problems which arise in oil exploration, and 3) Study of the applications of nonlinear evolution equations. Work is underway to construct a model which can give a first approximation to the transport properties of fluid mixtures in their dependence on size and mass of the constituent particles. Work is also underway to develop and test various methods of estimating the number of oil pools in an area from a number of random drillings. The nonlinear evolution equations being investigated describe a very large number of energy related processes. One such equation, the so-called Sine-Gordon equation, has been under study and a number of previously unknown results for the equation have been found.

RUTGERS UNIVERSITY
Department of Mechanics and Materials Sciences
Piscataway, New Jersey 08854

49. STRESS CREEP OF STRUCTURAL METALS — $0 — 01-04, 81-3

G. J. Weng

This research is concerned with the study of creep behavior of structural metals at elevated temperature. As creep deformation involves both microstructural changes and macroscopic descriptions, this problem has been studied from both metallurgical and mechanics standpoints. These traditional studies however have been carried out independently. Starting from the consideration of microstructural activities, the object of this research program is to develop a physically-based method to describe the overall, macroscopic creep behavior of materials. We have established the basic framework of this approach, and applied it to examine the creep activity of metals under fatigue loading. It was found that, due to the change of microstructures, the creep deformation of metals is greatly accelerated under the influence of cyclic loading. Upon fractional unloading, both creep acceleration and retardation may be resulted, the actual behavior being dependent on the fraction and the extent of creep deformation at which cyclic loading is imposed. The effect of fatigue loading has also been examined under a strain-controlled process. It was further found that due to the accelerated creep and additional alternating strain, the relaxation of mean stress is greatly enhanced. All these results indicate that in the design and analysis of structural members at elevated temperature, the material properties should not be taken from a simple static test, but should be done directly from the cyclic or dynamic tests, if the materials are likely to encounter fatigue loading.

SANDIA NATIONAL LABORATORIES
Device Research Division
Albuquerque, New Mexico 87185

50. HIGH TEMPERATURE ELECTRONICS — $100,000 — 01-03, 80-6
R. J. Chaffin, L. R. Dawson
D. R. Myers, T. E. Zipperian

This project addresses fundamental engineering questions relevant to the development of high-temperature (up to 500°C) electronics for energy technologies. Included are sensors, passive components, and active semiconductor devices which provide electronic gain. The work has concentrated on electronic devices fabricated from gallium phosphide (GaP), aluminum gallium arsenide ($Al_xGa_{1-x}As$), and heterojunctions formed from gallium phosphide and aluminum gallium phosphide ($GaP/Al_xGa_{1-x}P$). A $GaP/Al_xGa_{1-x}P$ heterojunction bipolar transit P heterojunction bipolar transistor has shown useful transistor action from -195 C to 550°C and a $GaP/Al_xGa_{1-x}P$ heterojunction, semiconductor-controlled rectifier has demonstrated useful solid-state switching to 550°C. These are the highest operational temperatures ever recorded for such devices. Initial results from this project have shown that it is feasible to build active solid-state semiconductor devices. Initial results from this project have shown that it is feasible to build active solid-state semiconductor devices for high-temperature service. Future plans include developing stable metallization systems for these devices and developing device geometries and processing techniques compatible with a high-temperature integrated circuit technology.

SANDIA NATIONAL LABORATORIES
Combustion Sciences Directorate
Thermofluids Division
Livermore, California 94550

51. CONVECTIVE DROPLET VAPORIZATION AND COMBUSTION — $150,000 — 01-05 81-3

B. R. Sanders, H. A. Dwyer,
A. R. Kerstein,

The technical goal of this project is to develop a complete analysis of liquid droplet vaporization and combustion processes through single droplet modeling and a statistical approach to multidroplet interactions. First, an analysis of liquid droplet vaporization and combustion will be developed by solving the coupled shear-driven recirculation flow within the droplet and the external convective gas-phase flow past the droplet, where a differential velocity exists between the droplet and free stream. Second, a statistical approach will be developed to study the combustion of a large ensemble of droplets whose locations and sizes are randomly distributed. The detailed solution of individual droplet heating and vaporization will be used as empirical inputs to the statistical spray combustion model. The single droplet numerical model has been extended to include variable transport properties in liquid and gas phases, complete separated fluid mechanics, and mass transport at the droplet surface. Additionally, a combusting spray was modeled where droplet interactions influence the connectedness of the flame zone (localized pockets of flame vs. a single connected continuum). Percolation theory has been used to identify the transition between these regimes, and to derive the dynamics of this transition as burnout proceeds in a simple spray geometry. This is the first known application of statistical methods to the problem of flame zone connectedness, a previously unresolved question of long standing.

SCIENTIFIC SYSTEMS, INC.
54 Rindge Avenue Extension
Cambridge, Massachusetts 02140

52. CHAOTIC DYNAMICS IN FEEDBACK SYSTEMS $25,000 01-03
J. Baillieul, R. W. Brockett 82-3
N. Kopell

The objective of this research effort is to study chaotic motions occuring in certain classes of dynamical systems which arise in the study of feedback control systems, electric power conversion circuitry and various other engineering applications. Part of the effort is focused on a simple class of differential equations whose coefficients depend piecewise linearly on the state. Because this is a simpler class of dynamical systems than others (such as the well known Lorenz system) which have been widely studied recently, it is possible to obtain especially accurate simulations of system trajectories. On the other hand, numerical simulations that have been carried out indicate very interesting qualitative features of the dynamics of such systems, and there is evidence of a strange attractor in a very simple third order system. Specific research is aimed at these and other classes of models in three areas: (i) the use of singular perturbations techniques to analyze first return maps, (ii) the use of difference equations to study to qualitative behavior of "chaotic" differential equations, and (iii) the use of input/output analysis (particularly various control theoretic techniques involving Nyquist plots, describing functions, etc.) to study the qualitative behavior of feedback models.

SKF INDUSTRIES, INC.
Technology Services Division
1100 First Avenue
King of Prussia, Pennsylvania 19406

53. LUBRICATION OF ENGINEERING SURFACES - II — $0 — 01-01, 80-3
J. I. McCool

The objective is to refine the prediction of the traction in lubricated rolling/sliding/spinning contacts to account for the effect of anisotropic roughness and lubricant parameters. Issues investigated include:

1) Sources of error in stylus profile measurements, e.g. finite stylus radius, stylus dynamics and quantization error.

2) Criteria for setting filter limits in roughness signal processing.

3) Effect of errors in microcontact models such as the assumed mechanical independence of asperities and multi-variate gaussian distribution of surface slopes and curvatures.

Software models have developed for simulating microcontact behavior (area, force and contact density) and macrocontact behavior (film thickness, traction). An optical rig is used for measuring traction and lubricant film thickness.

UNIVERSITY OF SOUTHERN CALIFORNIA
Department of Physics
University Park
Los Angeles, California 90089

54. A STUDY OF GAS-SURFACE ENERGY EXCHANGE PROCESSES — $63,000 — 01-02 83-3
J. A. Kunc, D. E. Shemansky

The objective of this theoretical research program is to study the fundamental characteristics of gas-surface energy exchange reactions. The interaction process refers to low density conditions in the gas component and therefore has general application to a number of diverse disciplines, such as atmospheric evolution of exospheric planetary bodies, the study of orbital characteristics of artificial satellites, the maintenance of clean high vacuum systems for research in subjects such as fusion reactions, and many other important areas in engineering and technology. The approach to the calculations is to construct accurate theoretical models of the solid structure on a microscopic scale, and account for the many body gas-surface physical interaction using Monte Carlo techniques. The project is presently at the stage of testing the program in 60 dimensional He - Alpha quartz, and H - Alpha quartz interaction systems in which entrappment, adsorption and scattering events are accumulated to describe the aggregate interaction probabilities.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Division of Applied Mechanics
Stanford, California 94305

55. ENERGY CHANGES IN TRANSFORMING SOLIDS — $150,000 — 01-04, 82-4

George Herrmann, David M. Barnett
A. Golebiewska-Herrmann

Energy changes in deformable solids accompany and control a variety of processes related to void formation, void growth, damage and fracture. A powerful method for characterizing such changes is based on material conservation and balance laws. The basic quantity of interest in this connection is the so-called material momentum tensor, which plays a role analogous to the stress tensor. Several problems have been recently completed and are currently under study. They include calculation of energy changes associated with boundaries and interfaces, introducing the concept of material traction, analogous to (classical) physical (or spatial) Cauchy traction, and investigating a variety of geometries. Another problem concerns the properties of the material momentum itself. In linear elasticity, this quantity is asymmetric. It is established, however, that in a fully nonlinear theory, this tensor is symmetric and proper linearization leads to a new symmetric material momentum even in classical linear elasticity, whose properties have yet to be fully explored.

The calculation of the redistribution of impurity atoms about a uniformly gliding edge dislocation is currently being performed. The local impurity concentration is governed by a non-linear diffusion equation which must be solved by finite difference techniques; the source of non-linearity is essentially due to the fact that only one impurity atom is allowed to occupy any given substitutional site. Once the concentration variation is obtained, the solute drag force on the dislocation can be determined from Lothe's power dissipation theorem. We then intend to study solute redistribution near a uniformly climbing edge dislocation and near dislocations in non-uniform motion.

We have succeeded in developing a proper prescription for defining chemical potential at the interface between two dissimilar stressed elastic solids; this prescription accounts for differences in specific volumes of the two media and is valid for quite general stress states. We have begun to examine the relationship between our expression for chemical potential and the "force on an interface" as first deduced by Eshelby.

STANFORD UNIVERSITY
Edward Ginzton Laboratory
Stanford, California 94305

56. HIGH FREQUENCY TRANSDUCERS — $97,000 — 01-03, 81-3
G. S. Kino

This year, a new theory has been developed for cross-coupling in acoustic transducer arrays, used for acoustic imaging. Cross-coupling changes the pulse response and the angular response of the arrays. The results compare very well with theory. This is an entirely new theoretical technique applicable to acoustics devices for NDT, medical and sonar arrays, as well as to electromagnetic and antenna arrays. Techniques for reducing cross-coupling have also been suggested and tried with some success.

New developments have been made of air transducers operating at 1 and 2 MHz in air. These are used for precision measurements of distance in air. This is of great importance for diamond turning, robotic applications, nondestructive testing and profile measurements in precision manufacturing.

STANFORD UNIVERSITY
Mechanical Engineering Department
Stanford, California 94305

57. A NEW METHOD FOR PREDICTING MULTIAXIAL FATIGUE DAMAGE — $66,000 — 01-04, 81-3

D. V. Nelson

The objective of this project is to develop an improved method for predicting the fatigue life of components which experience multiaxial cyclic straining. Using available data in the literature, an evaluation of existing methods used in design analysis (e.g., the procedures of the ASME Boiler and Pressure Vessel Code) showed that they are often non-conservative when loadings are applied out-of-phase, which is frequently the case in service. The evaluation also showed that two new approaches are more accurate than existing ones as well as being conservative. The first approach predicts life based on maximum shear strain amplitude modified by a fraction of the normal strain amplitude acting on the plane(s) which experiences the multiaxial cyclic plastic work to life, using only uniaxial fatigue and cyclic stress-strain properties as input to the computations. Of the two new approaches, the plastic work method appears somewhat superior, and a test program is underway to provide a critical check of it. Specimens of A533B pressure vessel steel are being tested in deflection-controlled, combined bending and torsion, applied both in-phase and 90 degrees out-of-phase, at two different fixed ratios of bending-to-torsion strain, and at a number of different strain amplitudes to produce lives ranging between 10^2 to 10^6cycles. The life to formation and subsequent growth of cracks from 0.1 mm size till fracture (10 mm size) are being recorded. Based on test results to date, it appears that the relative fatigue damage of in-phase vs. out-of-phase loading, as well as crack growth behavior, depends on both the bending-to-torsion ratio and the strain amplitudes being applied. Thus far, the plastic work approach is correlating experimental trends with reasonably good success.

STANFORD UNIVERSITY
Department of Chemistry
Stanford, California 94305

58. EFFICIENCY OF CHEMICAL AND THERMAL ENGINES — $92,000 — 01-06 82-4
J. Ross

Research is focussed on the issue of the possibility of increasing the power output of thermal and chemical engines by means of external perturbations. The power output of an engine is necessarily accompanied by dissipation due to the presence of irreversible processes. We have investigated and find the possibility of an increase in power output of a thermal engine, driven by a chemical reaction, by means of external periodic variation of a thermodynamic constraint for the same chemical throughput as the unperturbed (steady or periodic) state. An increase in power output is accompanied by a decrease in the rate of entropy production. The increased efficiency is achievable due to the nonlinearities in the system and resonance effects. Research is planned on optimization of cycles for combined thermal and chemical engines, and the search for upper limits of the efficiency of chemical engines with nonzero throughput (reaction rates) of monotonic and oscillatory reactions.

STANFORD UNIVERSITY
Department of Civil Engineering
Stanford, California 94305

59. MOMENTUM AND HEAT TRANSFERS IN A COMPLEX, BUT WELL-DEFINED TURBULENT FLOW — $80,000 — 01-02, 81-3

R. L. Street

A basic study of a three-dimensional, variable density, recirculating flow being conducted in a lid-driven cavity. A unique facility has been created to provide an extremely well-regulated flow. Water is the working fluid. The objectives of the research are to provide 1) a complete data base for a range of conditions (laminar, turbulent, forced convection, etc.) in a complex recirculating flow, 2) deeper insight into the physical processes governing heat and momentum transport in such flow, and 3) a critical evaluation of the performance of numerical simulation models in predicting the experimental results. Flow visualization has been carried out for flows in which the fluid is either 1) homogeneous or 2) stably stratified. General flow features have been established for Reynolds numbers up to 10,000, e.g., the number of identifiable eddy structures, the presence of Taylor-Gortler-type (TGT) vortices, and the strength and the development of the thermocline in the stratified cases. Direct heat flux measurements and LDA measurements of velocities are being made. Comparison has been made with both two- and three-dimensional numerical codes. Some codes fail to represent accurately the flow because of defects in their formulations. However, several correctly formulated codes do reproduce the experimental results for laminar flows quite well, except for the TGT vortices which are not found in the numerical results. Turbulent flow cases and code modifications are to be examined.

STANFORD UNIVERSITY
Mechanical Engineering Department
Stanford, CA 94305

60. HEAT TRANSFER EFFECTS OF LONGITUDINAL VORTICES EMBEDDED IN A TURBULENT BOUNDARY LAYER — $50,000 — 01-02 82-3

John Eaton

Longitudinal vortices embedded in boundary layers occur in a number of flow situations, such as Taylor-Gortler vortices on concave surfaces or horseshoe vortices formed at a surface protuberance. In spite of the occurence of these vortices in devices for which heat transfer is important, very little research has been done to isolate their influence on heat transfer rates. Both single longitudinal vortices and vortex pairs will be embedded in a flat plate turbulent boundary layer using simple vortex generators. Detailed fluid-dynamic data and spatially resolved heat transfer data will be obtained. The construction and qualification of the wind tunnel has been completed including computer controlled traversing. The constant heat flux test surface is installed and is presently being qualified. The surface is capable of resolving surface heat transfer variations with a spatial resolution of approximately 1/10 of the boundary layer thickness.

SYSTEMS ENGINEERING FOR POWER, INC.
4300 Evergreen Lane, 302
Annandale, Virginia 22003-3211

61. SPATIAL CORRELATION FACTORS IN WIND ENERGY SYSTEMS — $0 — 01-03, 81-3
G. L. Blankenship

Two aspects of the dynamics of wind energy systems have been considered in this study. Both are related to the impacts of spatial correlation in the variations of the wind energy distribution on the dynamical behavior of wind turbine systems. In the first case the distribution of an array of wind turbines over a large, contiguous area raises the possibility of energy exchanges among the machines through electromechanical interconnections in response to random variations in the space-time distribution of wind energy. The potential destabilizing effect of non-uniform energy distributions under both transient and steady state conditions is of special interest. It has been shown that certain coupling geometries promote energy exchanges, and hence instabilities, and that others have the reverse effect. A simulation program which represents the dynamics of a three machine MOD-2 system similar to the current installation in Washington state has been implemented and tested using on-site wind data. Theoretical work on the dynamics of stochastic arrays has led to the development of a technique for estimating the aggregate output of a large array of regularly spaced dynamical systems responding to random inputs and parametric disturbances. In the second part of this study the effects of local turbulence in the wind flow on the dynamics of a single wind turbine have been examined. Given the blade dimensions (150-300 ft.) and flexibilities associated with large turbines and other features of the turbine design, it is not unlikely that local, random variations in wind energy distribution across the swept area of the blades could induce oscillatory behavior in the blade dynamics. Assuming that the local turbulence fluctuations are random and rapidly varying, exact stochastic stability boundaries have been computed for a linear model of the blade/wind dynamics. This work has been generalized to the treatment of stochastic stability problems in linear systems with general classes of parametric disturbances.

UNIVERSITY OF TEXAS AT AUSTIN
Center for Studies in Statistical Mechanics
Austin, Texas 78712

62. BIFURCATIONS AND FLUCTUATIONS IN FAR FROM EQUILIBRIUM SYSTEMS — $100,000 — 01-06, 81-3
Ilya Prigogine

In many instances, physico-chemical systems give rise to self-organization and complex behavior. Bifurcations and fluctuations constitute the basic mechanism of evolution far from thermodynamic equilibrium. The purpose of this research is to explore the implications of bifurcations and fluctuations in the modeling, design and stability of complex systems of interest in physics and engineering. Special emphasis is being placed on the following two aspects. First, the effects of temperature fluctuations on the performance of chemical reactors is being examined in connection with the onset of explosive behavior. Second, the coupling between a complex system and its environment is being considered. Previous work has shown the possibility of a new type of transition induced by environmental noise and external fields. The repercussion of these transitions is being studied for systems involving multiphotonic steps.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY
Depts. of Engineering Mechanics and Mechanical Engineering
Blacksburg, Virginia 24061

63. HEAT TRANSFER IN OSCILLATORY FLOW — $94,000 — 01-02, 82-4

D. P. Telionis, T. E. Diller

The response of the velocity field and heat transfer of a single cylinder and bundles of cylinders to forced oscillations of the mean stream is investigated. Parallel experiments are conducted in a wind tunnel and a water tunnel. In the first facility the emphasis will be given to heat transfer, whereas in the second the flow will be examined in detail via Laser-Dopple Velocimetry and Flow Visualization. Analytical efforts will be based on numerical integrations of boundary layer equations and special mathematical tools for modeling the flow and heat transfer is improved with simultaneous decrease of the flow resistance. Two unsteady wind tunnels have been designed, constructed and calibrated especially for this project. A water tunnel was modified accordingly to achieve independent control of amplitude and frequency. The first phase of heat transfer and pressure fluctuation data has been completed. Results indicate that the overall heat transfer increases with the amplitude of the oscillation. Finite-differencing techniques have been incorporated in a computer code which predicts successfully the flow and heat transfer in the attached boundary layer.

UNIVERSITY OF WISCONSIN
Department of Chemical Engineering
Madison, Wisconsin 53706

64. THE DEVELOPMENT OF PROCESS DESIGN AND CONTROL STRATEGIES FOR ENHANCED ENERGY EFFICIENCY IN THE PROCESS INDUSTRIES — $80,000 — 01-03, 80-6

M. Morari, W. H. Ray, D. F. Rudd

The process industries are a major consumer of energy and the improvement of energy efficiency is an important goal. Process modifications aiming at a reduction of energy consumption tend to make a plant more integrated and thus more difficult to operate. In practice, the primary objective is not only steady state energy efficiency but that the plant is flexible, operable and controllable, i.e. resilient. The research goals are to develop design strategies for resilient processes and operating policies for highly integrated plants. The particular subtasks are: 1) Synthesis of resilient energy management networks, 2) Development of control strategies for integrated distillation columns, and 3) Development of control and optimization procedures for systems with high parametric sensitivity (chemical reactors). The latter two tasks involve an extensive experimental verification phase. The development of interactive user-friendly CAD packages incorporating the fundamental theoretical developments are under way.

BUDGET NUMBER INDEX

Number

01-01
Includes projects concerned with research related to friction and wear. See project numbers:

8, 15, 34, and 53

01-02
Includes projects concerned with research on the effects of turbulence, vibrations and noise, and heat transfer. See project numbers:

2, 3, 5, 7, 10, 11, 16, 21, 22, 30, 36, 37, 38, 42, 44, 54, 59, and 63

01-03
Includes projects concerned with research on adaptive control systems, non-linear systems, modeling, sensors for hostile environments, and NDE instrumentation. See project numbers:

1, 6, 13, 18, 23, 24, 25, 28, 29, 31, 33, 35, 39, 43, 46, 50, 52, 56, 61, and 64

01-04
Includes projects concerned with research on the macroscopic aspects of elastoplastic deformations and of crack propagation in structural materials. See project numbers:

4, 19, 20, 45, 49, 55, and 57

01-05
Includes projects concerned with research on data bases, lean mixture ignitions, and modeling of real combustion systems. See project numbers:

12, 14, 27, 32, 40, 47 and 51

01-06
Includes projects concerned with research on analysis of non-imaging optics, and noise and fluctuations in non-linear systems. See project numbers:

9, 17, 26, 41, 48, 58 and 62

PROJECT TITLES

Budget Number		Project Number
01-01		
	THE EFFECT OF AIR FLOW INSIDE A PNEUMATIC TIRE ON TEMPERATURE BUILDUP AND ROLLING RESISTANCE	8
	ELECTROCHEMICAL WEAR MECHANISM AND DEPOSIT FORMATION IN LUBRICATED SYSTEMS	15
	PISTON PING FRICTION AND VEHICLE FUEL ECONOMY	34
	LUBRICATION OF ENGINEERING SURFACES - II	53
01-02		
	THEORETICAL/EXPERIMENTAL STUDY OF STABILITY CONTROL	2
	MITIGATION OF BIOFOULING USING SURFACE COATINGS	3
	TWO-PHASE FLOW RESEARCH	5
	FLOW AND HEAT TRANSFER IN UNIFORM AND NON-UNIFORM POROUS BEDS	7
	BURSTING IN STEADY AND PULSATING TURBULENT PIPE FLOW	10
	RADIATIVE HEAT TRANSFER IN OIL SHALE RETORTING	11
	FLUID MECHANICS OF ACOUSTIC RESONANCE IN HEAT EXCHANGER TUBE BUNDLES	16
	CONDITIONS FOR DROPWISE CONDENSATION ON ELECTROPLATED GOLD	21
	INTERACTIONS BETWEEN FRICTION-INDUCED VIBRATION AND WEAR	22

PROJECT TITLES

Budget Number		Project Number
01-02		
	NUMERICAL MODELING OF TURBULENT ENERGY RELATED FLOWS	30
	HYDRODYNAMIC PREDICTION OF MULTIDIMENSTIONAL SINGLE-AND TWO-PHASE FLOW IN ROD ARRAY	36
	FLOW AND HEAT TRANSFER WITH IMPINGING JETS AND WALL JETS	37
	FUNDAMENTAL HEAT TRANSFER PROCESSES RELATED TO PHASE-CHANGE THERMAL STORAGE MEDIA	38
	CONVECTIVE BOILING HEAT TRANSFER IN NARROW ANNULAR GAPS	42
	HOLOGRAPHIC INVESTIGATION OF THERMAL-NONEQUILIBRIUM VAPOR GENERATION IN TWO-PHASE FLOWS	44
	A STUDY OF GAS-SURFACE ENERGY EXCHANGE PROCESSES	54
	MOMENTUM AND HEAT TRANSFERS IN A COMPLEX, BUT WELL-DEFINED TURBULENT FLOW	59
	HEAT TRANSFER EFFECTS OF LONGITUDINAL VORTICES EMBEDDED IN A TURBULENT BOUNDARY LAYER	60
	HEAT TRANSFER OF OSCILLATORY FLOW	63
01-03		
	A COMPOSITE MULTIVIEWING TRANSDUCER	1
	IMPROVEMENT IN THE DESIGN AND EXTENSION OF OPERATING RANGE OF VISCOMETERS AND THERMAL CONDUCTIVITY CELLS	6
	COMBUSTION CONTROL WITH SMART SENSORS	13
	CRACK CHARACTERIZATION WITH ULTRASONIC NDE	18

PROJECT TITLES

Budget Number		Project Number
01-03		
	METHOD OF VIBRATIONAL CONTROL IN THE PROBLEM OF STABILIZATION OF CHEMICAL REACTORS.....	23
	BASIC DATA FOR THE DEVELOPMENT OF MOLECULES AS THRESHOLD ELECTRON DETECTORS.....	24
	THIN FILM CHEMICAL SENSORS BASED ON ELECTRON TUNNELING.....	25
	PROCESSING AND CHARACTERIZATION OF SCATTERED SIGNALS FROM ACOUSTIC TARGETS.....	28
	DEVELOPMENT OF INTEGRATED THERMIONIC CIRCUITS..	29
	SHORT-CUT PROCEDURES FOR THE SIMULTANEOUS DESIGN OF A PROCESS AND ITS CONTROL SYSTEMS....	31
	A STUDY OF REDUCED ORDER MODEL REFERENCE CONTROL SYSTEMS FOR IMPROVED PROCESS CONTROL...	33
	IMPROVEMENT OF RELIABILITY OF WELDING BY IN-PROCESS.....	35
	THERMOPHYSICAL PROPERTIES OF HYDROCARBON MIXTURES	39
	EFFECTS OF CRACK GEOMETRY AND NEAR-CRACK MATERIAL BEHAVIOR ON SCATTERING OF ULTRA-SONIC WAVES FOR ONDE APPLICATIONS.....	43
	HIGH TEMPERATURE CHEMICALLY SENSITIVE ELECTRONIC DEVICES.....	46
	HIGH TEMPERATURE ELECTRONICS.....	50
	CHAOTIC DYNAMICS IN FEEDBACK SYSTEMS.....	52
	HIGH FREQUENCY TRANSDUCERS.....	56
	SPATIAL CORRELATION FACTORS IN WIND ENERGY SYSTEMS.....	61

PROJECT TITLES

Budget Number		Project Number
01-03		
	THE DEVELOPMENT OF PROCESS DESIGN AND CONTROL STRATEGIES FOR ENHANCED ENERGY EFFICIENCY IN THE PROCESS INDUSTRIES.....	64
01-04		
	DAMAGE ACCUMULATION BY CRACK GROWTH UNDER COMBINED CREEP AND FATIGUE.....	4
	ENGINEERING ANALYSIS OF ELASTIC-PLASTIC FRACTURE.....	19
	CONTINUOUS DAMAGE THEORY.....	20
	CRACK-TIP FIELDS FOR MATERIALS WITH EXPONENTIAL LAW CREEP BEHAVIOR AT HIGH STRESS.....	45
	STRESS CREEP OF STRUCTURAL METALS.....	49
	ENERGY CHANGES IN TRANSFORMING SOLIDS.....	55
	A NEW METHOD FOR PREDICTING MULTIAXIAL FATIGUE DAMAGE.....	57
01-05		
	MEASUREMENT AND CORRELATION OF HEAT TRANSPORT PROPERTIES FOR MODEL COAL LIQUID COMPOUNDS USING AN EXISTING HOT WIRE INSTRUMENT.....	12
	FUNDAMENTAL HIGH PRESSURE DROPLET COMBUSTION CHARACTERISTICS OF EMULSIONS, MIXTURES AND SLURRIES.....	14
	CONTROLLED COMBUSTION.....	27
	TURBULENT PREMIXED FLAME STUDY.....	32

PROJECT TITLES

Budget Number		Project Number
01-05		
	SUPPORT OF CRITICAL DATA COMPILATIONS.....	40
	MEASUREMENT AND PREDICTION OF LIQUID MIXTURE THERMAL CONDUCTIVITY AND VISCOSITY.....	47
	CONVECTIVE DROPLET VAPORIZATION AND COMBUSTION.....	51
01-06		
	FUNDAMENTALS AND TECHNIQUES OF NONIMAGING OPTICS FOR SOLAR ENERGY CONCENTRATION	9
	PREDICTIVE MODELING OF URANIUM ROLL TYPE DEPOSITS.....	17
	STUDIES IN NONLINEAR DYNAMICS	26
	TOPICS IN PHSICO-CHEMICAL DYDRODYNAMICS.....	41
	SOME BASIC RESEARCH PROBLEMS RELATED TO ENERGY	48
	EFFICIENCY OF CHEMICAL THERMAL ENGINES.....	58
	BIFURCATIONS AND FLUCTUATIONS IN FAR FROM EQUILIBRIUM SYSTEMS	62

Abarbanel, D. I. 31
Achenbach, J. D. 48
Ajello, J. M. 29
Alajajian, S. 29
Avedisian, C. T. 19
Baier, R. E. 8
Baillieul, J. 57
Bankoff, S. G. 47
Barna, B. A. 23
Barnett, D. M. 60
Bassani, J. L. 50
Bates, J. M. 49
Beck, T. R. 20
Berger, B. S. 35
Bernard, P. S. 35
Blankenship, G. L. 66
Blevins, R. D. 21
Brenden, B. B. 49
Brockett, R. W. 57
Case, K. M. 53
Catton, I. 12
Chaffin, R. J. 55
Chen, S. S. 7
Cheng, W. 37
Chutjian, A. 29
Cohen, E. G. D. 53
Corones, J. 6
Creer, J. M. 49
Daniel, J. L. 49
Dawson, L. R. 55
Diller, T. E. 68
Dooley, R. 34
Douglas, J. M. 36
Dwyer, H. A. 56
Eaton, J. 65
Fornalik, M. S. 8
Goldstein, R. J. 42
Golebiewska-Herrmann, A. 60
Graboski, M. S. 17
Gucinski, H. 8
Hardt, D. E. 38
Hardt, D. E. 40
Herrmann, G. 60
Hoult, D. P. 39
Jaske, C. E. 9
Jendrzjczyk, J. A. 7
Johnson, J. A. 23
Jones, M. C. 16
Kalpakjian, S. 27
Kaufman, A. N. 31
Keck, J. 37
Keiser, D. D. 23
Kerstein, A. R. 56
Kestin, J. 11
Khanna, S. K. 30
King, R. W. 8
Kino, G. S. 61
Kopell, N. 57
Krajcinovic, D. 25
Kunc, J. A. 59
Lambe, J. 30
Lauks, I. R. 51
Levich, B. G. 46
Lide, D. R. 45
Lynn, D. 34
Malone, M. F. 36
Masubuchi, K. 40
Maxfield, B. 33
McCool, J. I. 58
McCormick, B. 34
McLaughlin, J. B. 15
Meerkov, S. M. 28
Meyer, A. E. 8
Miller, E. 33
Morari, M. 69
Myers, D. R. 55
Nelson, D. V. 62
Nunge, R. J. 15
O'Gallagher, J. 14
Olien, N. 44
Oppenheim, A. K. 32
Ortoleva, P. J. 22
Paynter, H. M. 40
Pope, S. 37
Prigogine, I. 67
Rae, W. J. 13
Raveche, H. J. 44
Ray, W. H. 69
Reiss, E. L. 7
Reuter, W. G. 24
Rife, J. M. 39
Robinson, J. T. 41
Ross, J. 63
Rovner, D. M. 10
Rowley, R. L. 52
Rudd D. F. 69
Sanders, B. R. 56
Seydel, J. A. 23
Shemansky, D. E. 59
Skinner, G. T. 13

Sloan, E. D. 17
Sparrow, E. M. 43
Street, R. L. 64
Tankin, R. S. 47
Telionis, D. P. 68
Thompson, D. O. 6
Todreas, N. E. 41
Tow, D. M. 23
Unkel, W. C. 40
Wei, J. 51
Weng, G. J. 54
Westwater, J. W. 26
Wilde, D. 34
Winston, R. 14
Wolga, G. L. 18
Yuen, M. C. 47
Yuen, S. 51
Zemel, J. N. 51
Zipperian, T. E. 55

I. Geosciences Research Program

1. What is the detailed budget structure of the Geosciences Research Program? What types of work are funded by each of these budget categories?

Answer: The Geosciences Research Program is divided into four broad categories:

Geology, Geophysics and Earth Dynamics
Geochemistry
Energy Resource Recognition, Evaluation and Utilization
Solar-Terrestrial/Atmospheric Interactions

The kinds of work funded under each of these categories is detailed on pages xi, xii and xiii of DOE/ER-0145/1, "Summaries of Physical Research in the Geosciences," copies of which are attached.

2. For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
GEOSCIENCES RESEARCH

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
OPERATING EXPENSES					
GEOLOGY, GEOPHYSICS AND EARTH DYNAMICS	$ 4329	$ 3387	$ 3631	$ 3380	$ 3713
GEOCHEMISTRY	2315	3171	4193	4000	4419
ENERGY RESOURCE RECOGNITION, EVALUATION AND UTILIZATION	1661	2038	3276	4220	4573
SOLAR-TERRESTRIAL/ ATMOSPHERIC INTERACTIONS	789	836	798	1050	975
CAPITAL EQUIPMENT	932	899	890	960	1100

3. For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of Geosciences funding going to DOE laboratories.

Answer: Please see the table below for requested information.

INTRODUCTION TO THE GEOSCIENCES RESEARCH PROGRAM OF THE OFFICE OF BASIC ENERGY SCIENCES

The Geosciences Research Program is directed by the Department of Energy's Office of Energy Research, within the Office of Basic Energy Sciences, Division of Engineering, Mathematical, and Geosciences. Research supported by this program may be directed toward a specific energy technology, national security, conservation of the environment, or the safety objectives of the Department of Energy. The purpose of this program is to develop geoscience or geoscience-related information relevant to one or more of these Department of Energy objectives or to develop a broad, basic understanding of geoscientific materials and processes necessary for attaining long-term Department of Energy goals. In general, individual research efforts supported by this program may involve elements of all four objectives.

The Geosciences Research Program is divided into five broad categories:

- Geology, geophysics, and earth dynamics
- Geochemistry
- Energy resource recognition, evaluation and development
- Hydrologic and marine sciences
- Solar-terrestrial-atmospheric interactions.

The following content outline of these categories is intended to be illustrative rather than exhaustive, and will evolve with time. Individual research efforts at the Department of Energy, university, college, corporate, not-for-profit, and other Federal agency laboratories supported by this program frequently have components in more than one of the categories or subcategories listed.

I. Geology, Geophysics, and Earth Dynamics

A. Large-Scale Earth Movements. Research related to the physical aspects of large-scale plate motion, mountain building, and regional scale uplift or subsidence.

B. Evolution of Geologic Structures. Research bearing on the history and development of geologic structures (e.g., folds, faults, landslides, and volcanoes) on a local or subregional scale.

C. Properties of Earth Materials. Research on physical properties of rocks and minerals determined in the laboratory or in the field (in situ) by direct or indirect techniques.

D. Rock Flow, Fracture, or Failure. Research related to response of minerals, rocks, and rock units to natural or artificially induced stress, including the strain rates that range from those appropriate to drilling to viscoelastic response.

E. Continental Scientific Drilling Program (CSDP). Research on advanced technology and services as well as scientifically motivated projects concerned with utilizing shallow (0.3 km), intermediate (0.3 to 1 km), and deep (1 km to 9 km) drill holes in the United States continental crust to (a) obtain samples for detailed physical, chemical, mineralogical, petrologic, and hydrologic characterization and interpretation; (b) correlate geophysical data with laboratory-determined properties; and (c) use the drill hole as an experimental facility for studying crustal materials and processes. The Department of Energy focuses on drilling through an active hydrothermal system (or systems) into a magma chamber or into high-temperature igneous rocks. Research includes aspects of drilling technology development for such hostile environments. Part of a multiagency (U.S. Geological Survey, National Science Foundation, Department of Energy, and Department of Defense) coordinated program.

2. Geochemistry

   A. Thermochemical Properties of Geologic Materials. Research related to thermodynamic, physical, and transport properties of natural geologic materials and their synthetic analogues. Emphasis is on generic rather than site-specific studies.

   B. Static Rock-Water Interactions. Laboratory-based research on chemical, mineralogical, and textural consequences of interaction of natural aqueous fluids, or their synthetic analogues, with rocks and minerals.

   C. Organic Geochemistry. Research on naturally occurring carbonaceous and biologically derived substances of geologic importance, including research on the origin and development of coal, petroleum and gas.

   D. Geochemical Migration. Research on chemical migration in materials of the earth's crust, emphasizing a generic rather than specific understanding, which may (ultimately) lead to predictive capability. These experimental and theoretical studies focus on chemical transport induced by pressure, temperature, and composition gradients within, between, and by a phase or phases. This component is part of a multiagency (Department of Energy, National Science Foundation, U.S. Geological Survey) joint program.

3. Energy Resource Recognition, Evaluation, and Development

   A. Resource Definition and Utilization. The principal goal of this research is to develop new and advanced techniques that are physically, chemically, and mathematically based, for energy and energy-related resource exploration, definition, and use.

   B. Reservoir Dynamics and Modeling. Research related to dynamic modeling of geothermal and hydrocarbon reservoirs in their natural and perturbed (by production, injection, or reinjection) states.

   C. Magma Energy Resources. Field, laboratory, experimental, and theoretical research bearing on the origin, migration, emplacement, and crystallization of natural silicate liquids or their synthetic analogues. These studies emphasize the extraction of energy from such liquids.

   D. Information Compilation, Evaluation, and Dissemination. These research activities are principally oriented toward evaluating existing geoscientific data to identify significant gaps, including the necessary compilation and dissemination activities.

4. Hydrologic and Marine Sciences

   A. Ground Water Hydrology. Research related to chemical and physical principles underlying the flow of water through porous and permeable rocks near the earth's surface.

   B. Fresh Water Systems. Research on the chemistry, physics, and dynamics of fresh water systems, including streams, rivers, and lakes.

   C. Oceanography. Research involving materials and processes of the marine environment. Principal emphasis is on geological, geophysical, and geochemical research related to rocks and sediments beneath the water column.

5. Solar-Terrestrial-Atmospheric Interactions

A. Magnetospheric Physics and Chemistry. Research directed toward developing a fundamental understanding of the interactions of the solar wind with the terrestrial magnetic field. Research related to the earth's magnetosphere as a model magnetohydrodynamic generator and associated plasma physics research.

B. Upper Atmosphere Chemistry and Physics. Research on thermal, compositional, and electrical phenomena in the upper atmosphere, and the effects induced by solar radiation.

C. Solar Radiation. Research on the solar constant, spectral distribution, and characteristics of solar radiation of the earth, including the long-term effects of solar radiation on the climate.

D. Meteorology and Climatology. Interrelationships of weather and climate with energy systems.

BASIC ENERGY SCIENCES
GEOSCIENCES RESEARCH

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0403 GEOSCIENCES					
KC0403010 GEOLOGY, GEOPHYSICS AND EARTH DYNAMICS					
OPERATING EXPENSES					
LAWRENCE BERKELEY LAB	$ 350	$ 325	$ 330	$ 414	$ 321
LAWRENCE LIVERMORE NAT LAB	595	380	480	640	610
LOS ALAMOS NATIONAL LAB	805	200	338	315	450
SANDIA CORP	350	805	375	360	373
KC0403020 GEOCHEMISTRY					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	310	330	330	360	373
LAWRENCE BERKELEY LAB	385	495	756	645	759
LAWRENCE LIVERMORE NAT LAB	150	230	205	250	259
LOS ALAMOS NATIONAL LAB	410	705	801	940	894
OAK RIDGE NATIONAL LAB	380	430	430	470	486
PACIFIC NORTHWEST LABS	170	100	100	105	109
SANDIA CORP	0	185	280	318	329
KC0403030 ENERGY RESOURCE RECOGNITION, EVALUATION AND UTILIZATION					
OPERATING EXPENSES					
LAWRENCE BERKELEY LAB	245	260	319	390	316
LAWRENCE LIVERMORE NAT LAB	315	169	595	875	749
LOS ALAMOS NATIONAL LAB	45	405	305	715	615
PACIFIC NORTHWEST LABS	85	95	95	115	119
SANDIA CORP	885	556	1027	1262	1305
KC0403040 HYDROLOGIC AND MARINE SCIENCES					
OPERATING EXPENSES					
LAWRENCE BERKELEY LAB	95	100	0	0	0
LAWRENCE LIVERMORE NAT LAB	0	38	0	0	0
KC0403050 SOLAR - TERRESTRIAL/ ATMOSPHERIC INTERACTIONS					

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
OPERATING EXPENSES					
LOS ALAMOS NATIONAL LAB	165	165	240	330	341
PACIFIC NORTHWEST LABS	325	325	325	350	361
35KC04000					
CAPITAL EQUIPMENT					
AMES LABORATORY	88	20	50	95	20
ARGONNE NATIONAL LAB	142	155	190	180	30
IDAHO NATIONAL ENG LAB	54	0	40	20	20
LAWRENCE BERKELEY LAB	285	225	610	280	120
LAWRENCE LIVERMORE NAT LAB	113	370	200	180	120
LOS ALAMOS NATIONAL LAB	265	205	180	170	150
OAK RIDGE NATIONAL LAB	196	285	135	190	290
PACIFIC NORTHWEST LABS	116	55	55	110	70
SANDIA CORP	252	190	100	120	130
SANDIA LAB, LIVERMORE	0	30	0	0	0

4. **For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of Geosciences funding going to universities.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
GEOSCIENCES RESEARCH

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0403 GEOSCIENCES					
KC0403010 GEOLOGY, GEOPHYSICS, AND EARTH DYNAMICS					
OPERATING EXPENSES					
ALASKA UNIV OF	$ 70	$ 0	$- 23	$ 0	$ 0
ARIZONA UNIV OF	60	60	48	0	0
BROWN UNIV	164	165	400	0	196
CALIF UNIV OF BERKELEY	144	150	165	196	181
CALIF UNIV OF DAVIS	0	0	- 5	0	0
CALIF UNIV OF LOS ANGELES	167	0	60	126	72
COLUMBIA UNIV	318	318	337	359	351
HAWAII UNIV OF	0	88	96	105	109
MASSACHUSETTS INST TECH	260	257	263	257	290
MINNESOTA UNIV OF	68	0	0	0	0
NEW YORK CITY U - QUEENS	84	81	0	0	0
NEW YORK ST UNIV OF ALBANY	88	0	0	0	0
OREGON STATE UNIV	0	38	0	0	0
OREGON UNIV OF	0	0	103	0	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
PENNSYLVANIA STATE UNIV	83	0	0	0	0
RENSSELAER POLYTECHNIC	91	99	150	0	98
RICE WILLIAM MARSH UNIV	0	0	120	130	134
SOUTH FLORIDA UNIV OF	30	0	0	0	0
SOUTHERN METHODIST UNIV	54	70	0	0	0
STANFORD LELAND JR UNVR	140	125	160	170	176
TEXAS A&M UNIV	202	200	201	163	155
WISCONSIN UNIV OF	0	0	- 6	48	0
YALE UNIV	35	26	39	45	47
KC0403020 GEOCHEMISTRY					
OPERATING EXPENSES					
ARIZONA STATE UNIV	62	66	123	0	62
CALIF UNIV OF BERKELEY	0	0	203	0	104
CHICAGO UNIV OF	0	38	98	0	52
COLUMBIA UNIV	150	156	289	0	155
MINNESOTA UNIV OF	0	57	0	65	67
NEW YORK ST UNIV OF ST BROOKE	65	- 2	112	120	124
SOUTH DAKOTA SCH OF MINES	0	67	100	90	93
STANFORD LELAND JR UNVR	0	91	101	107	114
TULSA UNIV OF	75	71	75	80	82
WOODS HOLE OCNOGRAPH INST	139	150	190	208	207
KC0403030 ENERGY RESOURCE RECOGNITION, EVALUATION AND UTILIZATION					
OPERATING EXPENSES					
CALIFORNIA INST OF TECH	0	0	72	80	82
HARVARD UNIV	0	0	372	0	191
NEVADA UNIV OF	0	75	87	95	98
NEW YORK STATE U - QUEENS	0	0	49	0	0
NEW YORK ST UNIV OF ALBANY	0	39	136	0	62
TEXAS UNIV OF	0	0	54	0	0
WISCONSIN UNIV OF	36	0	0	0	0
KC0403050 SOLAR-TERRESTRIAL/ ATMOSPHERIC INTERACTIONS					
OPERATING EXPENSES					
ALASKA UNIV OF	108	113	132	120	129
ARIZONA UNIV OF	96	98	101	110	114

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
35KC04000					
CAPITAL EQUIPMENT					
NEW YORK UNIV	250	250	260	200	0
WISCONSIN UNIV OF	9	0	0	0	0

5. **For the period FY 1981 - FY 1985, please provide, by budget category and by company, the amount of Geosciences Research funding going to industry.**

Answer: Please see the table below for requested information.

BASIC ENERGY SCIENCES
GEOSCIENCES RESEARCH

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC0403 GEOSCIENCES					
KC0403030 ENERGY RESOURCE RECOGNITION, EVALUATION AND UTILIZATION					
OPERATING EXPENSES					
WOODWARD-CLYDE CONSULTANTS	$ 0	$ 100	$ 100	$ 100	$ 100
XDATA CORP.	0	54	66	66	66
35KC0400					
CAPITAL EQUIPMENT					
XDATA CORP.	0	14	0	0	0

6. **For the period FY 1981 - FY 1985, please provide, by budget category and by agency, the amount of Geosciences Research funding going to other agencies.**

Answer: No funds in the Geosciences research program are provided to other agencies.

7. **What is the Continental Scientific Drilling Program (CSDP)? When was it initiated? What agencies are participating?**

Answer: The CSDP is a cooperative interagency scientific study of the structure, composition, evolution and dynamics of the continental crust which utilizes drilling as the key to the third dimension of the earth's crust. The effort bears strongly on the mission objectives of the DOE, USGS and NSF.

After a 15 year gestation period in the scientific community, the first funding to an effort identified as CSDP was provided by the Department of Energy in FY 1979. The initial efforts were as a 4-agency informal cooperation--DOE, NSF, DOD and USGS. DOD support has been minimal and a formal "Accord" (attached) is being put in place by DOE, NSF and the USGS.

AN INTERAGENCY ACCORD
ON
CONTINENTAL SCIENTIFIC DRILLING
BY
DEPARTMENT OF ENERGY
(Represented by the Office of Energy Research)
DEPARTMENT OF THE INTERIOR
(Represented by the U.S. Geological Survey)
AND
NATIONAL SCIENCE FOUNDATION

I. Essential Purpose

a. Each of these Federal agencies (Participating Agencies), in line with statutorily chartered responsibilities, has been and continues to be directly concerned with continental drilling for scientific and engineering studies.

b. The Participating Agencies intend, by this Accord, to ensure that their respective interests in a number of ongoing and future Federal scientific activities involving continental scientific drilling are appropriately coordinated.

c. The coordinated continental scientific drilling activity described in this document will avoid undesirable duplication or gaps in federal scientific efforts toward achieving better basic understanding of the processes that, operating through time, have led to the evolution of the chemical and physical structure and properties of the earth's continental crust. These goals of these activities contribute directly to the solution of serious national problems such as ensuring adequate supplies of energy, water and mineral resources, safe isolation of wastes, protection against the hazards of earthquakes and volcanic eruptions, and national defense.

II. Principal Interests and Basic Responsibilities of Participating Agencies

a. Department of Energy (DOE):

1. DOE's interests in continental scientific drilling include fundamental research on the thermal regimes of the earth's crust, enhanced utilization of geothermal, fossil and nuclear energy resources in a safe and environmentally sound manner, and effective fulfillment of national security responsibilities.

2. DOE interests include thermally driven crustal processes in the formation and utilization of energy resources, in the safe disposal of waste products from geothermal energy processes, in fossil and nuclear energy processes, in nuclear test containment, and in the reliable use of seismic waves for treaty verification. DOE is also well aware of the importance of scientific study of the transition zone between magmas and their associated hydrothermal circulation systems within the thermal regime domains of the earth's crust.

3. In view of DOE's significant mission-related interests, and its pertinent Laboratory resources and expertise, DOE's contributions to the continential scientific drilling activity can be expected to include primary responsibility for the logistics of drilling in thermal regime areas and for the support of a substantial portion of the R&D related thereto.

b. U.S. Geological Survey (Survey) of the Department of the Interior:

1. The interest of the Survey in the continental scientific drilling activity stems from its mission to pursue fundamental knowledge of the geology of the Nation in its many aspects by carrying out the full spectrum of scientific and technical activities in the geological field. The Survey's interests also pertain to its scientific and technical role in national Policy decisions on the optimum use and management of the Nation's land, energy, mineral, and water resources, and for the mitigation of geological hazards.

2. The Survey's participation in the continental scientific drilling activity is to achieve objectives in direct support of Mineral and Energy Resource programs and Geohazards programs related to volcanic and earthquake activity. The objectives are integrated into an overall effort directed toward a better understanding of the deep continental crust; these include deep drilling into mineralized fossil and active hydrothermal systems, drilling to understand both ancient and active forces deforming the continental crust, and drilling to obtain a better understanding of the structure and chemistry of the continental crust and upper mantle.

c. National Science Foundation (NSF):

1. NSF's interest in the continental scientific drilling activity follows from its national role in the support of basic scientific research and in strengthening scientific research potential in a broad spectrum of scientific fields. Drilling is an especially important tool for the scientific exploration of the earth's crust. Continental scientific drilling will complement the Foundation's current activities in ocean drilling and in the geological, geophysical and geochemical study of the continental crust.

2. NSF's role in continental scientific drilling is: 1) to support, selectively, basic research involving down-hole instrumentation and core studies utilizing drill holes funded by the NSF or other sources; 2) to support, when appropriate, the drilling and/or deepening of holes to help answer basic questions on the structure and evolution of the continental crust; 3) to cooperate with other agencies involved to ensure proper management and coordination of the program, through, for example, the support of conferences, workshops. and curatorial facilities.

III. Contents of the Continental Scientific Drilling Activity

a. The Participating Agencies expect that, from time to time during the existence of this Accord, they will agree upon specifically identified

projects, conducted or to be undertaken by one or more of the Participating Agencies that they deem should be considered part of the continental scientific drilling activity. Each such project shall be defined in writing and may be in the form of an implementing written supplement to this Accord, identifying the project and containing such additional information bearing on the respective roles of the Participating Agencies or other facets as these agencies agree are necessary or desirable.

b. Each implementing written supplement hereto, and this Accord, may be revised at any time or times in writing by the participating agencies.

c. The continental scientific drilling activity shall consist only of those projects or activities that are designated by the Participating Agencies pursuant to a. and b., above.

IV. Functioning of Participating Agencies

a. In relation to continental scientific drilling projects, or any potential continental scientific drilling project, representatives, designated by the participating agencies, shall meet, from time to time, as and when agreeable, and in any event at least quarterly. Such designees shall constitute the Interagency Coordinating Group for Continental Scientific Drilling.

b. At such meetings, and in connection with other discussions among Participating Agencies relative to this Accord, each of the Participating Agencies shall be represented by such officials or employees as it designates.

c. Informal discussions among Participating Agencies relative to this Accord shall be encouraged, and meetings shall be conducted with such formality or informality as the attending designated representatives of the Participating Agencies deem appropriate.

d. The Participating Agencies recognize that, from time to time, it may be advantageous to the objectives of this Accord to obtain outside advice from knowledgeable organizations or individuals, and to include other Executive Branch entities as Participating Agencies. It is further recognized that an effective effort in continental scientific drilling will require not only cooperation by the Participating Agencies but also communicative links with the entire geoscience community.

e. All decisions in implementation of the provisions of this Accord must be made unanimously to be considered binding on the Participating Agencies, except as said Agencies may otherwise stipulate in writing in certain instances; provided, however, that any of the Participating Agencies may, by written notice to the others, withdraw from the continental scientific drilling activity any project which it is conducting.

f. Any of the Participating Agencies may withdraw from participation under this Accord by written notice to the others. This Accord shall be considered terminated at any time that there are less than two Participating Agencies.

V. Predominating Factors -

a. This Accord and its implementations are and will be subject to all applicable legal requirements and responsibilities pertaining to the respective Participating Agencies.

b. It is expected that the implementing written supplements to this Accord referred to in Section III., above, will be arrived at in light of not only the legally obtaining circumstances mentioned in a., above, but also the prevailing and forseeable budgetary, contractual, and other practicalities affecting each of the Participating Agencies.

c. Though this Accord is essentially a statement of intention and purpose, rather than a legally binding instrument, the Participating Agencies believe that effective implementation of this cooperative arrangement will enhance the prospect of scientific and technical contributions to a number of national missions.

DATED: _____, 1983

Department of Energy
BY: Office of Energy Research

_____
(Title)

Department of the Interior
BY: U.S. Geological Survey

_____
(Title)

National Science Foundation
By:

_____
(Title)

8. What have been the funding levels of the CSDP, by agency, since the program's initiation?

Answer:

(Obligations in Millions)

Agency	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984
DOE/BES	.4	1.5	2.2	3.1	4.1	4.9
DOE/GHTD	.08	0	0	0	0	5.9
DOD	0	.01	.01	.01	.01	?
NSF	0	.03	.03	.03	.4	.4
USGS	0	.06	.07	.07	.07	.08
Total	.48	1.59	2.31	3.21	4.48	11.28

9. **How does the research funded by the Geosciences Research Program differ, complement, supplement, or overlap geosciences research funded by other DOE programs and by other agencies such as the National Science Foundation or the U.S. Geological Survey?**

Answer: The Geosciences Research Program of the Office of Basic Energy Sciences supports long-range, basic and generic research at DOE laboratories, universities and industry in areas of the geosciences that are relevant to the nation's present and future energy needs. The BES Geosciences program is characterized by an emphasis on basic and applied research in energy-related areas of the geosciences which are too long-range or too high-risk to be included in the research activities of the DOE technology programs.

The multi-technology relevance of these basic research efforts can often justify support of a long-range study in a BES program which would not be of sufficient urgency to justify support by any one technology program. For example, the downhole geophysical instrumentation required to operate in the hostile environment to be encountered in the CSDP deep drilling studies in thermal regimes, such as high heat flow measurements, sets this program apart from the complementary DOE efforts by, for example, the Division of Geothermal and Hydropower Technology and the Office of Civilian Radioactive Waste Management whose technological goals are more immediate and applied. Focus on the nation's energy needs is a clear DOE responsibility which guides the BES Geosciences Research Program into those areas of long-range, basic research not otherwise supported by the National Science Foundation, with its broad science mandate, or the U.S. Geological Survey with its emphasis on geological studies by in-house scientists of mineral, water and land resources and earthquake and volcanic hazards.

10. **What types of formal and informal advisory groups does the Division of Engineering and Geosciences to assure that the Geosciences Research Program is of high quality and coordinated with the research carried out at other agencies? If any formal advisory groups exist, please provide a listing of the current membership.**

Answer: Research proposals submitted to the Geosciences Program are sent out for independent review by peer scientists whose recommendations are weighed heavily in the decision process. Peer reviewers are selected for their eminence in the field and for an absence of any conflict of interest in the outcome. All decisions to fund are systematically subject to signed approval by the BES staff of trained scientists which reviews the written justifications for project funding against the criteria of scientific merit and originality and appropriateness to the DOE/BES mission. In addition, site visits and project reviews are carried out periodically by the Geosciences Program staff.

The Geosciences Program staff meet regularly with key DOE laboratory staff to help assure the maintenance of the highest quality Geosciences research in the DOE laboratories. Periodic reviews of the major university projects help to assure the continued high quality of that effort and helps stimulate university scientists to interact with those in the DOE laboratories in areas of mutual interest.

The Geosciences Program interacts with six different NAS/NRC committees to help set priorities and guide the research support into those areas of the highest scientific merit. The Continental Scientific Drilling Program, for example, is coordinated informally with the scientific community through the activities of the NAS/NRC Continental Scientific Drilling Committee.

Coordination with other agencies which support research in the geosciences (DMA, DARPA, NASA, NOAA, NRC, NSF, USGS) is achieved through the Interagency Geophysics Discussion Group, an informal group of representatives from these agencies who meet on a regular monthly schedule to discuss geoscience topics of mutual interest, including program coordination.

11. What has DOE done towards planning an enhanced Geosciences program?

Answer: The Department of Energy is not proposing substantial enhancement of the BES Geosciences program nor has it established any plan for future enhancements. As part of normal program management, candidate efforts are formulated in some detail and considered each year as substitutes for or additions to current efforts. Over the past five years, the program has been modified and has grown to accommodate a number of specific initiatives designed to further DOE technology objectives:

- Geochemical Migration in the Earth's Crust
- Rock Mechanics
- Continental Scientific Drilling
- Organic Geochemistry
- Basic Studies Relating to Nuclear Waste Isolation

During the next budget cycle, it is expected that the principal candidates under discussion will be additional research in organic geochemistry, which underpins many aspects of use of fossil energy resources, and initiation of deeper drilling for scientific purposes at one or two sites selected for the insight they can give into thermal regimes, i.e., the coupled transport of mass and energy in the continental crust.

12. What funding levels would be required to conduct such an enhanced program?

Answer: The discussions expected during the next budget cycle will no doubt consider a variety of possible funding levels for the Geosciences program, including both increases and decreases from the level proposed in FY 1985.

13. Please provide a copy of the latest Geosciences research summaries.

Answer: A copy of DOE/ER-0145/1, "Summaries of Physical Research in the Geosciences," dated September, 1983 is attached. Additional copies are available on request. The 1984 edition is anticipated by the end of the summer.

546

Summaries of Physical Research in the Geosciences

September 1983

FOREWORD

The Department of Energy supports research in the geosciences in order to provide a sound foundation of fundamental knowledge in those areas of earth, atmospheric, and solar-terrestrial sciences that are germane to the Department of Energy's many missions. The Division of Engineering, Mathematical and Geosciences -- part of the Office of Basic Energy Sciences which is under the Director of Energy Research -- supports the Geosciences Research Program. The participants in this program include the major Department of Energy laboratories, industry, universities, and other governmental agencies. Such support, formalized by a contract between the Department of Energy and the organization performing the work, provides funds for salaries, equipment and other materials, and an overhead allowance.

The summaries in this document, prepared by the investigators, describe the scope of the individual programs and detail the research performed during 1982-1983. The Geosciences Research Program includes research in geology, petrology, geophysics, geochemistry, hydrology, solar-terrestrial relationships, aeronomy, seismology, and natural resource analysis, including the various subdivisions and interdisciplinary areas. All such research is related either directly or indirectly to the Department of Energy's technological needs.

INTRODUCTION TO THE GEOSCIENCES RESEARCH PROGRAM OF THE OFFICE OF BASIC ENERGY SCIENCES

The Geosciences Research Program is directed by the Department of Energy's Office of Energy Research, within the Office of Basic Energy Sciences, Division of Engineering, Mathematical, and Geosciences. Research supported by this program may be directed toward a specific energy technology, national security, conservation of the environment, or the safety objectives of the Department of Energy. The purpose of this program is to develop geoscience or geoscience-related information relevant to one or more of these Department of Energy objectives or to develop a broad, basic understanding of geoscientific materials and processes necessary for attaining long-term Department of Energy goals. In general, individual research efforts supported by this program may involve elements of all four objectives.

The Geosciences Research Program is divided into five broad categories:

- Geology, geophysics, and earth dynamics
- Geochemistry
- Energy resource recognition, evaluation and development
- Hydrologic and marine sciences
- Solar-terrestrial-atmospheric interactions.

The following content outline of these categories is intended to be illustrative rather than exhaustive, and will evolve with time. Individual research efforts at the Department of Energy, university, college, corporate, not-for-profit, and other Federal agency laboratories supported by this program frequently have components in more than one of the categories or subcategories listed.

I. Geology, Geophysics, and Earth Dynamics

A. Large-Scale Earth Movements. Research related to the physical aspects of large-scale plate motion, mountain building, and regional scale uplift or subsidence.

B. Evolution of Geologic Structures. Research bearing on the history and development of geologic structures (e.g., folds, faults, landslides, and volcanoes) on a local or subregional scale.

C. Properties of Earth Materials. Research on physical properties of rocks and minerals determined in the laboratory or in the field (in situ) by direct or indirect techniques.

D. Rock Flow, Fracture, or Failure. Research related to response of minerals, rocks, and rock units to natural or artificially induced stress, including the strain rates that range from those appropriate to drilling to viscoelastic response.

E. Continental Scientific Drilling Program (CSDP). Research on advanced technology and services as well as scientifically motivated projects concerned with utilizing shallow (0.3 km), intermediate (0.3 to 1 km), and deep (1 km to 9 km) drill holes in the United States continental crust to (a) obtain samples for detailed physical, chemical, mineralogical, petrologic, and hydrologic characterization and interpretation; (b) correlate geophysical data with laboratory-determined properties; and (c) use the drill hole as an experimental facility for studying crustal materials and processes. The Department of Energy focuses on drilling through an active hydrothermal system (or systems) into a magma chamber or into high-temperature igneous rocks. Research includes aspects of drilling technology development for such hostile environments. Part of a multiagency (U.S. Geological Survey, National Science Foundation, Department of Energy, and Department of Defense) coordinated program.

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   A. Thermochemical Properties of Geologic Materials. Research related to thermodynamic, physical, and transport properties of natural geologic materials and their synthetic analogues. Emphasis is on generic rather than site-specific studies.

   B. Static Rock-Water Interactions. Laboratory-based research on chemical, mineralogical, and textural consequences of interaction of natural aqueous fluids, or their synthetic analogues, with rocks and minerals.

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   D. Geochemical Migration. Research on chemical migration in materials of the earth's crust, emphasizing a generic rather than specific understanding, which may (ultimately) lead to predictive capability. These experimental and theoretical studies focus on chemical transport induced by pressure, temperature, and composition gradients within, between, and by a phase or phases. This component is part of a multiagency (Department of Energy, National Science Foundation, U.S. Geological Survey) joint program.

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   A. Resource Definition and Utilization. The principal goal of this research is to develop new and advanced techniques that are physically, chemically, and mathematically based, for energy and energy-related resource exploration, definition, and use.

   B. Reservoir Dynamics and Modeling. Research related to dynamic modeling of geothermal and hydrocarbon reservoirs in their natural and perturbed (by production, injection, or reinjection) states.

   C. Magma Energy Resources. Field, laboratory, experimental, and theoretical research bearing on the origin, migration, emplacement, and crystallization of natural silicate liquids or their synthetic analogues. These studies emphasize the extraction of energy from such liquids.

   D. Information Compilation, Evaluation, and Dissemination. These research activities are principally oriented toward evaluating existing geoscientific data to identify significant gaps, including the necessary compilation and dissemination activities.

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   A. Ground Water Hydrology. Research related to chemical and physical principles underlying the flow of water through porous and permeable rocks near the earth's surface.

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   C. Oceanography. Research involving materials and processes of the marine environment. Principal emphasis is on geological, geophysical, and geochemical research related to rocks and sediments beneath the water column.

5. Solar-Terrestrial-Atmospheric Interactions

A. Magnetospheric Physics and Chemistry. Research directed toward developing a fundamental understanding of the interactions of the solar wind with the terrestrial magnetic field. Research related to the earth's magnetosphere as a model magnetohydrodynamic generator and associated plasma physics research.

B. Upper Atmosphere Chemistry and Physics. Research on thermal, compositional, and electrical phenomena in the upper atmosphere, and the effects induced by solar radiation.

C. Solar Radiation. Research on the solar constant, spectral distribution, and characteristics of solar radiation of the earth, including the long-term effects of solar radiation on the climate.

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CONTENTS

FOREWORD

INTRODUCTION TO THE GEOSCIENCES RESEARCH PROGRAM OF THE OFFICE OF BASIC ENERGY SCIENCES

PART I. ON-SITE 1

ARGONNE NATIONAL LABORATORY 2

Geosciences Program 2

A. Thermochemistry of Geothermal Materials 2
B. Trace-Element Transport in Geologic Media 2
C. Migration of Heavy Element Chemical Species in Geologic Strata 3

LAWRENCE BERKELEY NATIONAL LABORATORY 5

Geosciences Program 5

A. Nonisothermal Reservoir Dynamics 5
B. Thermodynamics of High Temperature Brines 6
C. Rock-Water Interactions 6
D. Thermodynamic Properties of Silicate Liquids 6
E. Chemical Transport in Natural Systems 7
F. Aqueous Solutions Data Base 8
G. Deep Electromagnetic Sounding of the Crust 8
H. Effect of Fracture Characteristics upon Sonic Wave Propagation in Boreholes 9
I. Center for Computational Seismology (CCS) 9
J. Site Studies and Downhole Samplers: Continental Scientific Drilling Program 10
K. Asteroid Impacts and Mass Extinctions 10
L. Fluid Flow in Stressed Rock 11
M. Generation and Migration of Petroleum and its Precursor Compounds 11

LAWRENCE LIVERMORE NATIONAL LABORATORY 12

I. Geology, Geophysics, and Earth Dynamics 12

A. Rock Mechanics 12
B. Diffusion in Silicate Materials 12
C. Electrical Conductivity and Temperature in Upper Mantle 13
D. Attenuation and Dispersion in Partially Saturated Rocks 13
E. Surface Wave Method for Determining Earthquake Mechanisms with Applications to Regional Stress Field Studies 13

II. Geochemistry 14

A. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions 14
B. Kinetic and Compositional Model of High-Pressure Kerogen Pyrolysis 15

III. Energy Resource Recognition, Evaluation and Utilization
Continental Scientific Drilling Program: Thermal Regimes 16

A. Continental Drilling Program Information and Data Management Unit 16
B. Underground Imaging 17
C. Viscosity and Electrical Conductivity of Rock Melts: Continental Scientific Drilling Program 17
D. Thermal and Petrologic Studies of Large Silicic Systems 17
E. CSDP: Imperial Valley Information Base 18

LOS ALAMOS NATIONAL LABORATORY 19

I. Geophysics 19

A. Creep Deformation of Rocks 19
B. Radiative Heat Transfer in Minerals, Glasses, and Melts 20
C. Electrical Conductivity and Temperature in the Upper Mantle 20
D. Nonlinear Generation of Acoustic Beams 21

II. Geochemistry 22

A. Rock-Water Interaction in Geothermal Systems 23
B. Element Migration and Fixation in Crustal Rocks 23
C. Physiochemical Basis of the Na-K-Ca Geothermometer 23
D. Cation Site Size and Coulomb Energy Calculations for the Principal Rock-Forming Minerals 24
E. Coal Research: Occurrence, Form, and Distribution of Sulfur in Peat 24
F. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures 25
G. Geochemistry of Technetium and Geochemical Controls on the Redistribution of Multivalent Elements in the Lithosphere 25

III. Thermal Regimes and Continental Scientific Drilling Program 27

A. Field, Petrologic and Geochemical Studies of the Polvadera Group, Jemez Mountains, New Mexico 27
B. Origin and Extent of the Toledo Caldera, Jemez Mountains, New Mexico, and its Relation to the Valles Caldera 28
C. Anomalous Lithospheric and Asthenospheric Structure Beneath the Valles Caldera/Rio Grand Rift of New Mexico 28
D. Valles Caldera Information Base 29

IV. Space Plasma Physics 30

A. Energy Transport in Space Plasmas 30
B. Electrodynamical Aspects of the Solar Wind-Magnetosphere Interaction 31
C. Theory of Energetic Electron Acceleration and Precipitation from the Terrestrial Magnetosphere 31

OAK RIDGE NATIONAL LABORATORY 32

Geochemistry of Crustal Processes at High Temperatures and Pressures 32

A. Silicate Melt Geochemistry 32
B. Hydrothermal Geochemistry 33
C. Geochemical Modeling 35

PACIFIC NORTHWEST LABORATORY 36

I. Remote Sensing and Geoscience Data Analysis Methodology 36

A. Remote Sensing and Geoscience Data Base Expansion 36
B. Software Development and Testing 37
C. Application and Transfer and Geodata Capabilities 37

II. DOE Insolation/Aeronomy Observatory Aeronomy Studies 38

A. Insolation Studies 38
B. Aeronomy Studies 39

III. Chemical Migration by Contact Metamorphism in Granite - Carbonate Rocks 41

SANDIA NATIONAL LABORATORY 42

I. Magma Energy Research 42

II. Continental Scientific Drilling Program Thermal Regimes 43

A. CSDP - Thermal Geophysical Techniques 43
B. Magmatic Emplacement 43
C. CSDP - Mono Craters-Long Valley (CA) Site Assessment 44
D. CSDP - Drilling, Logging and Instrumentation 44
E. CSDP - Shallow Hole Investigation of Long Valley, Valles and Salton Sea Thermal Regimes 44
F. Thermal Regimes Research Drilling Office 45
G. Long Valley-Mono Craters (CA) Information Base 45

III. Geophysics Research 46

A. Crustal Strain 46
B. Time-Dependent Deformation and Fracture of Brittle Rock 46
C. Creep of Sodium Chloride 47
D. Natural Convection in Double-Diffusive Counter-Buoyant Systems 47

IV. Geochemistry Research 48

A. Hydrothermal-Magma Systems 48
B. Clay-H_2O Interactions 48

V. Advanced Concepts 49

A. Field Portable Gas Chromatograph 49
B. Mapping Damage Space in Rocks Using Acoustic Emission 49
C. Noble Metals 50

PART II. OFF-SITE 51

UNIVERSITY OF ALASKA 52

I. The Magnetic Field Annihilation and Applications 52

UNIVERSITY OF ARIZONA 53

I. Rock Deformation in Hydrothermal Systems 53

II. Solar Variability: Figure and Mean Diameter 54

A. Technical Developments 54
B. Observations 54
C. Theoretical Work 54

ARIZONA STATE UNIVERSITY 55

Silicate, Aluminosilicate and Borosilicate Melts:
Thermochemical Studies by High-Temperature Calorimetry 55

BROWN UNIVERSITY 56

Major Volcanic Centers: Magnetotelluric Studies 56

A. Thermal Processes Associated with Major Volcanic Centers 56
B. Physio-chemical Processes Associated with the
Genesis of Primitive Crust 57
C. Magnetotelluric/Magnetic Variation Field System 57
D. Theoretical Models of Electromagnetic Induction Phenomena 57

CALIFORNIA INSTITUTE OF TECHNOLOGY 59

In Situ Stress in Deep Boreholes 59

UNIVERSITY OF CALIFORNIA AT BERKELEY 60

Isotopic Studies on Rare Gases in Terrestrial Samples
and in Natural Nucleosynthesis 60

Advective-Diffusion/Dispersion Transport
of Chemically Reacting Species 62

UNIVERSITY OF CALIFORNIA AT LOS ANGELES 63

Adiabats and Grüneisen Parameter at High Temperatures and Pressures 63

UNIVERSITY OF CHICAGO 64

Water and Magma Bodies 64

COLUMBIA UNIVERSITY 65

I. Tectonics of the Eastern Aleutian Arc 65

II. Fluid Transport Properties of Rock Fracture 66

HARVARD UNIVERSITY 67

Energetics and Thermochemical Properties of Rocks and Minerals 67

UNIVERSITY OF HAWAII AT MANOA 68

Physical Characterization of Magma Samples 68

MASSACHUSETTS INSTITUTE OF TECHNOLOGY 69

Seismology of Crack Formation 69

Microcrack Technology 70

UNIVERSITY OF MINNESOTA 71

Experimental Formation of Chalk from Calcareous Ooze 71

NATIONAL ACADEMY OF SCIENCES/NATIONAL RESEARCH COUNCIL 72

I. Studies in Geophysics 72

II. Committee on Seismology 74

III. U.S. National Committee for Geochemistry 75

IV. U.S. Geodynamics Committee 77

V. Continental Scientific Drilling Committee 80

VI. Geological Sciences Board 82

UNIVERSITY OF NEVADA 85

Studies of Magma Chambers in the Western Great Basin 85

A. Seismic Network Operation 85
B. Data Analysis 85
C. Interpretation 86

STATE UNIVERSITY OF NEW YORK/ALBANY 87

I. Thermal Evolution of Sedimentary Basins 87

II. Crustal Stretching and Subsidence in Sedimentary Basins 88

STATE UNIVERSITY OF NEW YORK/STONY BROOK 89

Geochemistry and Origin of Dolomites 89

RENSSELAER POLYTECHNIC INSTITUTE 90

Deep-burial Diagenesis in Carbonates 90

RICE UNIVERSITY 91

Structural Evolution of Central Brooks Range, Alaska 91

SOUTH DAKOTA SCHOOL OF MINES AND TECHNOLOGY 92

Thermally Induced Chemical Migration in Carbonate Rock 92

40-574 O - 85 - 36

STANFORD UNIVERSITY 93

I. Porosity with Fluids 93

II. Mechanism of Zeolite Crystallization and Alteration in Silicate Gasses 94

III. The Hydrothermal Solubility of Uraninite 95

TEXAS A&M UNIVERSITY 96

Mechanical and Transport Properties of Rocks 96

A. The Physical Nature of Fracturing at Depth 96
B. Fracture Permeability of Crystalline Rocks as a Function of Temperature, Pressure, and Hydrothermal Alteration 96
C. Mechanical Properties of Rocks at High Temperatures and Pressures 97

THE UNIVERSITY OF TEXAS AT AUSTIN 99

Investigation of a Fossil Geothermal System, Hamblin-Cleopatra Volcano, Clark County, Nevada 99

UNIVERSITY OF TULSA 100

Stability of Natural Gas in the Deep Subsurface 100

WOODS HOLE OCEANOGRAPHIC INSTITUTION 101

Organic Geochemistry of Outer Continental Margin and Deep Ocean Sediments 101

WOODWARD-CLYDE CONSULTANTS.....102

Earthquake Analyses: Long Valley/Mono Crater.....102

A. Reflected and Converted Phases from the Long Valley Magma Body 102
B. Source Mechanics of the Larger Earthquakes in the Long Valley Region 102
C. Analysis of Local Seismicity Data 103

XDATA CORPORATION 104

Computerized Underground Image Reconstruction 104

YALE UNIVERSITY 105

Opening Mode Crack Growth in Rock 105

GEOSCIENCES RESEARCH (AEC/ERDA/DOE) (HISTORICAL SUMMARY).....106

SUBJECT INDEX 108

INDEX OF TECHNICAL CONTRIBUTORS 109

PART I

ON-SITE

Contractor: ARGONNE NATIONAL LABORATORY
Argonne, Illinois 60439

Contract: 109 ENG 38

Title: Geosciences Program

Persons in Charge: F. A. Cafasso and M. J. Steindler

A. Thermochemistry of Geothermal Materials (P. A. G. O'Hare and G. K. Johnson)

This program has as its objective accurate determinations of thermodynamic quantities of zeolites and related minerals. Calorimetric measurement techniques available for these studies include the following: enthalpy of combustion and reaction, low-temperature heat capacity, drop calorimetry, and differential scanning calorimetry. The temperature range of interest is from $T \to 0$ to the upper temperature limit of stability, typically about 500 K. The selection of substances to be studied is determined not only by their actual or potential technological importance but also by attempts to relate the thermodynamic results to aspects of structure and bonding in aluminosilicates.

In this connection, our recent results for the entropies of analcime (Si/Al=2), natrolite, mesolite, and scolecite (Si/Al=1.5) suggest that in some of the zeolites the structure of the zeolitic water is "ice-like," while in others it is somewhat closer to that of "liquid-water." Results of X-ray diffraction studies have been used to deduce the configurational entropy of our specimen of natrolite. Comparison of experimental equilibrium measurements with our thermodynamic calculations suggests that $\Delta_f H^\circ$ (albite) may be in error.

Our current studies are concerned with heulandite and mordenite and future work will deal with chabazite, clinoptilolite, and erionite. Because of doubts about the validity of currently accepted thermodynamic quantities for albite, we will determine the complete thermodynamic properties of a highly ordered specimen as functions of temperature.

B. Trace-Element Transport in Geologic Strata (M. G. Seitz)

Migration of elements in geologic bodies is important in many situations. For example, migration has produced ores of benefit to man. Understanding ore-forming processes can improve our exploration capabilities for valuable mineral resources. Because element migration can disrupt inadequate schemes of waste disposal, the understanding of migration obtained in this program can aid in developing technically sound plans for the safe disposal of nuclear and chemical wastes.

In this study, the transport of elements by aqueous flow through geologic media is being examined principally by hydrothermal infiltration experiments in which groundwaters are pumped through rock cores to cause the movement of trace elements. The experiments are done at elevated pressures and at temperatures from 20 to 325°C to investigate migration processes typical of those in the upper crust of the earth.

The infiltration experiments are used because they yield valuable information concerning reaction kinetics, reaction reversibility, and the behavior of different chemical species in rock formations. Migration is observed directly; thus, the uncertainty in extrapolating data on a wide variety of chemical reactions to predict element movement in geologic settings is avoided. The results of specific experiments are generalized to many geologic situations by our efforts to establish continuity between experimental observations and theoretical predictions from transport models.

Using methods similar to those employed in the infiltration experiments, we are extracting pore fluids from rock cores mined from various depths in the earth and analyzing the fluids to obtain profiles of groundwater composition vs. depth in cored rock structures. This infiltration-sampling method has been demonstrated to be an effective tool for analyzing water in nearly impermeable rock, with the chemical profiles complementing data from water pumped directly from the holes. Dense, nearly impermeable rock is attractive for use in the disposal of nuclear waste.

Being investigated are the characteristics of metasomatism caused by groundwater infiltration and the effects of fulvic and humic acids on the mobilization and concentration of heavy metals in natural geologic settings.

C. Migration of Heavy Element Chemical Species in Geologic Media (S. M. Fried, A. M. Friedman, and F. Schreiner)

Our purpose in this program is to understand what the chemistry of the heavy elements is under geological conditions and how this chemistry affects the mobility of actinide species in geologic strata. The important chemical properties under investigation include oxidation-reduction, the nature and stability of complexes formed, solubility of compounds in groundwaters, self-diffusion in rock strata, and hydrolysis reactions. We are using spectrophotometric techniques to determine the distribution of oxidation states and calorimetric methods to determine equilibrium constants for hydrolysis and equilibrium reactions. Since the migration of the actinide elements from a geological repository will have an obvious dependence on their geochemistry, the results of these studies may be expected to be relevant to the evaluation of the safety of a radwaste repository.

Because basalt is a prime candidate for the emplacement of radwaste in a mined repository, we have continued our study of the interaction of basalt with hexavalent neptunium. We have found that basalt and its accompanying olivine are separately capable of reducing hexavalent neptunium to neptunium (V) and neptunium (IV). Most of the neptunium (IV) was found to deposit on the surface of the containers or the basalt; surprisingly the neptunium (V) formed by this reaction was also deposited on the surface of the mineral. It is hypothesized that the immobilization of a substantial amount of the neptunium (V) is the result of the formation of insoluble neptunyl (V) salts with some of the cationic components of the basalt and olivine (such as Al and Mg). We plan to study the properties of salts of this type, as well as developing methods to identify the particular compound on the rock surfaces.

In order to monitor the progress of chemical reactions of Np and Pu in dilute solutions, a commercial titration microcalorimeter has been modified so that heats of reaction of the order of 4 kilojoules per mole on amounts of the order of 10 micromoles of reactant may be measured. With this improved capability, complexing and hydrolysis reaction constants will be determined.

Contractor:	LAWRENCE BERKELEY LABORATORY University of California Berkeley, California 94720
Contract:	DE-AC03-76SF00098
Title:	Geosciences Program
Person in Charge:	T. V. McEvilly

Scope of Work

The geosciences program at LBL encompasses investigations in geochemistry, geophysics, reservoir dynamics, and applied geomechanics. Fundamental studies include the thermodynamic properties of silicate liquids and high-temperature brines, interactions between water and rock at elevated temperature and pressure, and the transport of fluid, heat, and chemically reactive solutes in groundwater systems. Geophysical activities encompass electromagnetic soundings of the crust, development and operation of a center for computational seismology, and an investigation of the effects of fracture characteristics on acoustic wave propagation in drill holes. The program is rounded out by hydrogeochemical studies in conjunction with the continental scientific drilling project and collection and evaluation of thermochemical data for use in assessment of the geologic disposal of nuclear wastes.

A. Nonisothermal Reservoir Dynamics (P. A. Witherspoon, C. F. Tsang and T. N. Narasimhan)

This project encompasses a wide range of fundamental studies in the fluid, heat and solute transport in underground formations. These studies have relevance to underground and other energy-related projects. The goal is to obtain a better understanding of various physical or chemical processes in porous or fractured media and their effects through analytic and numerical modeling.

More specifically, the following general topics are addressed:

1. Advanced well testing methods for fractured-porous media by means of coupled thermal, tracer and pressure measurements.

2. Development of a three-dimensional heat, fluid and solute transport code, based on the Integrated-Finite-Difference (IFD) technique. Generic studies of nonisothermal solute transport in idealized fracture or porous systems are made.

3. Continuation of the validation and applications of the LBL coupled thermo-hydromechanical model for fractured-porous media.

4. Development of a new integral form of the diffusion-type equation. This should make possible a reduction of mesh elements and the handling of moving boundary problems.

5. A fundamental study of the basis of the storage coefficient concept.

B. Thermodynamics of High Temperature Brines (K. S. Pitzer)

This project covers theoretical and experimental studies concerning the thermodynamic properties of aqueous electrolytes. The components important in natural waters and brines are emphasized. The resulting data are important in understanding certain geothermal and other natural resources. Moreover, this information has a wide range of applicability, since similar solutions arise in many industrial processes.

The experimental program involves measuring the heat capacity and the density of solutions in the range 0 to 300°C and 0 to 1 kbar. These measurements suffice to give a comprehensive equation of state, provided that other thermodynamic properties are known for a particular system at room temperature and pressure.

The theoretical work has yielded equations predicting the properties of mixtures based on the knowledge of the pure component solutions in water. In a number of cases, the calculated results for mixed brines are well verified by direct measurement. Phase equilibria can be predicted. Recent calculations have included a revised, general equation for all of the thermodynamic properties of aqueous NaCl to 300°C and 1 kbar as well as solubility calculations of Na_2SO_4 and several alkali halides in a variety of mixed electrolytes usually to about 250°C. Densities were measured recently for Na_2SO_4 and $MgSO_4$, and the heat capacity of the latter is now being measured. When these data are combined with earlier results, a comprehensive treatment can be given of phase equilibria over a range of temperatures for solutions containing the geochemically important ions Na^+, K^+, Mg^{++}, Ca^{++}, and Cl^-, $SO_4^=$, $HCO_3^=$, OH^-.

Other theoretical work concerns the properties of NaCl in high-pressure steam at temperatures to 800°C.

C. Rock-Water Interactions (J. A. Apps)

The objective of this project is to understand factors controlling albite solubility in aqueous solutions between 400°C and 0.1 to 50 MPa. The results are used in refining rock-water interaction models and data bases in order to model water-saturated rocks. The thermodynamic behavior of albite solubility measurements along the two-phase water saturation curve show that serious errors exist in the high temperature dissociation constants for the aqueous aluminum species, that current electrolyte models do not adequately account for ionic strength variations, and that the measurement of pH in quenched aqueous samples is subject to unpredictable error. Results are being evaluated to pinpoint the reasons for present difficulties.

D. Thermodynamic Properties of Silicate Liquids (I. S. E. Carmichael)

The objective of this research program is to better understand the properties of silicate liquids and their metastable quench products, silicate glasses. Ultimately these data will be used to interpret the generation and subsequent thermal history of natural silicate liquids.

The ultrasonic velocity and attenuation of a variety of silicate liquids has been measured to obtain their adiabatic compressibilities. In many liquids of low viscosity, the ultrasonic velocity is independent of frequency in the 3-12 MHz range and the velocity only increases slightly with temperature. For liquids of higher viscosity, the ultrasonic velocity is frequency-dependent, particularly at low temperatures, and the ultrasonic period may be shorter than the liquid relaxation time.

Using high-temperature drop calorimetry, the heat of fusion of $NaAlSiO_4$ has been measured, and in combination with measurements in other silicate liquids including those containing substantial amounts of both FeO and Fe_2O_3, values of partial molar oxide Cp's have been calculated. Fifty-three sets of data have been used in the regression with an average error of 3.5% which is almost twice the error of measurement. This is much larger than analogous oxide heat capacities in the corresponding low-temperature glasses where the error in the regression of 35 compositions is only 1.0%, barely more than the individual measurement error.

As silicate liquids cool, they transform to glasses. It is not yet possible to predict this transformation temperature for multicomponent liquids, but we have noted that if Fe_2O_3 is substituted for Al_2O_3 or Na for K, then the transition temperature is reduced.

A wide variety of natural silicate liquids was equilibrated in air above their liquidus temperatures (1200-1450°C), then quenched to glass, and analyzed for ferric and ferrous iron and for their other components. Data for 46 experiments were added to those obtained in previous years at much lower oxygen fugacities to give a regression equation relating the ferric-ferrous ratio in silicate liquids to temperature, oxygen fugacity, and composition.

E. Chemical Transport in Natural Systems (C. L. Carnahan)

The movement of chemically reactive solutes in natural groundwater systems under the influence of gradients of composition, temperature, and pressure is being investigated theoretically and numerically. The principal focus of this research is a full accounting of the irreversibility of such systems through application of the thermodynamics of irreversible processes. This approach allows consideration of thermodynamically coupled processes such as thermal diffusion (Soret effect), thermal osmosis, chemical osmosis, and coupled diffusion which cannot be treated by the traditional methods of equilibrium thermodynamics. Conservation equations and linear phenomenological equations have been formulated for the motion of a solution of electrolytes in a porous or fractured medium. The resulting time-dependent transport equations must be solved numerically because of the nonlinear relationship between chemical potentials and mass concentrations of solution components.

The current emphasis is on the behavior of thermodynamically open systems which have evolved to, or near, a nonequilibrium steady state. This state is characterized by a quantifiable, minimum rate of entropy production which is analogous to the minimum total Gibbs free energy of an isolated system in a state of equilibrium. The assumption of the steady state allows formulation of linear transport equations for many reacting systems; these equations are susceptible to solution analytically and are providing results of considerable interest.

F. Aqueous Solutions Data Base (S. L. Phillips)

This project publishes critically evaluated thermochemical data for use in the disposal of nuclear wastes in subsurface repositories; and, thermophysical data for modeling heat transport by aqueous solutions. Tables of recommended values are generated from correlating equations using computerized methods. The data used by this database are obtained mainly from published experimental values. Major emphasis now is on nuclear waste disposal.

Thermochemical properties for nuclear waste disposal include stability constants, solubilities, adsorption equilibria and Nernstian potentials to high temperatures, These data are for use in predicting the solubility and speciation of waste metals in salt, basalt and tuff repositories. A result of this project is identification of gaps where data are lacking or are inadequate, and recommendations for research to provide the needed data.

Besides critical evaluation of data, research is included on calculation of stability constants, solubilities and thermophysical properties to high temperatures; as well as computerized storage and retrieval of tables of data using desktop computers.

G. Deep Electromagnetic Sounding of the Crust (H. F. Morrison and N. E. Goldstein)

Variations in electrical conductivity within the crust are related mainly to the degree of connected porosity, saturation and salinity of pore fluids, as well as past or present thermal effects; e.g., temperature and hydrothermal alteration. Interpreted with thermal and seismic data, electromagnetic soundings might provide important information on thermal anomalies within the crust; including the existence of shallow magma bodies. The magnetotelluric (MT) method is the most common electromagnetic deep sounding method, but MT data from complex geological areas are often difficult to interpret accurately because distant inhomogeneities distort the electric fields at the point of measurement. To overcome this problem LBL developed a powerful controlled-source electromagnetic device for deep exploration. Because a dipole field is generated, depth of exploration is more limited than for MT, in which the excitation is provided by natural, ultra-low frequency plane waves. However, as the primary field strength of the dipole source decays according to an inverse cube of distance, the technique is less susceptible to distortions by inhomogeneities outside the region between the transmitter and receiver points.

Used together, MT and controlled-source EM methods provide a complementary data set. The LBL system is unique in that it has been designed for both types of soundings. Noise cancellation is achieved through use of a remote reference magnetometer, and in-field processing provides immediate reduction and display of data.

A mid-crustal conductor was detected and traced over a region of central Nevada between Winnemucca and Dixie Valley. This conductor is believed due to extension and heating of the crust beneath the Basin and Range province. In the Long Valley caldera, California, closely spaced stations in the south moat area delineated a shallow conductive feature that rises to within 2.5 km of the surface. The Long Valley caldera soundings were completed only days before the seismic swarm activity that began in mid-December 1982 and peaked in early January. Because there is a close spatial correlation between the conductivity anomaly and the earthquake hypocenters, the conductivity anomaly may be related to the magma injection that has been proposed to explain the seismicity. To test whether the conductivity anomaly is caused by a transient thermal pulse, we will carefully repeat selected soundings and perform numerical studies to relate conductivity changes to temperature changes caused by a simulated magmatic pulse.

H. Effect of Fracture Characteristics Upon Sonic Wave Propagation in Boreholes (M. S. King)

Fluid flow in rock is governed by the product of a single rock parameter, permeability, and the hydrological potential gradient existing in the rock mass. The determination of permeability is critical to any endeavor for which a knowledge of fluid flow is required. Such fields of interest lie in geothermal energy extraction, oil and gas recovery, deep crustal studies, energy storage in aquifers, and the storage of hazardous wastes. In rocks of low porosity, including many igneous, metamorphic and massive calcareous types, the in situ permeability is controlled by the presence of fractures rather than by the rock matrix permeability.

Geophysical borehole methods are available for detecting the presence of fractures adjacent to a borehole and therefore potentially for assessing the rock mass permeability in those cases that it is controlled by fractures. In particular, the borehole sonic log has shown considerable promise for locating fractures in rock. Field experiments are being conducted in which digitized sonic log waveforms are obtained across single, horizontal, isolated fractures intersecting a borehole in a crystalline rock mass. The fluid flow characteristics of these isolated fractures are measured using conventional borehole packer techniques, and the results compared. The field tests will be extended to zones in the same rock mass where systems of fractures intersect the borehole, and again the results of sonic and conventional packer tests will be compared. In this way it is anticipated that correlations will be established between such acoustic wave parameters as velocity and attenuation, and the permeability of the rock mass adjacent to the borehole.

I. Center for Computational Seismology (CCS) (T. V. McEvilly and E. L. Majer)

CCS was established to aid the computational seismologist in such matters as program development, data processing and display (graphics), and data management. CCS operates within a large computational facility (LBL computer center) and utilizes their resources as well as the expertise within the computer science and mathematics group of the physics division. These groups provide CCS with a valuable resource in hardware and software support. A goal of CCS is to make a wide variety of seismological and basic computational software available to the seismological community to maximize research dollars and time and avoid unnecessary duplication.

Consistent with these aims, CCS has acquired and implemented a state-of-the-art seismic reflection package for studies in seismic imagery. To date this package has been used to process and analyze data from geothermal environments (The Geysers, California; Cerro Prieto, Mexico; Grass Valley, Nevada) and for waste isolation studies (Hanford, Washington).

Other areas of study have included:

1. Structure of the San Andreas fault zone,
2. Mammoth Lakes, California seismic activity,
3. Source mechanism study of the Geysers earthquakes,
4. Synthetic seismographs in layered lossy media,
5. Differential tidal gravimetry (microgravimetry) for time-stress changes,
6. Near-field studies for source discrimination, and
7. Deep earth structure from $\tau - p$ inversion.

J. Site Studies and Downhole Sampler: Continental Scientific Drilling Program (J. M. Delany and A. F. White)

The main focus of this program is to evaluate the active hydrothermal system beneath the Valles caldera and lend support to the CSDP site evaluation process by generating a complete body of data to define the hydrothermal chemistry of the Baca reservoir. The data are used to determine to what extent, if any, geochemical components are introduced into the reservoir from a deeper magma/hydrothermal source. The use of existing deep holes drilled by industry in the Baca geothermal field, a known geothermal resource, has provided an efficient means of investigating the system's deep thermal fluids. A wellhead sampling program was completed in the fall of 1982. New fluid and gas samples have been collected from five deep Union Oil Company wells located in the Redondo Creek area. Standard and trace chemical analyses of waters and gases and isotopic analyses of water have been obtained. A comparison of these data from deep geothermal wells with analyses from surrounding hot springs and local groundwater may reveal if a signature of deeper hydrothermal fluids is present. In addition to sampling of fluids, drill cuttings from the same wells are being analyzed in order to assess the nature and extent of the water/rock interaction in the hydrothermal systems. This study is in collaboration with A. H. Truesdell (USGS) and John Reynolds (UC Berkeley) who will obtain major dissolved gas and isotopic concentrations and noble gas analyses, respectively, on the same samples.

K. Asteroid Impacts and Mass Extinctions (L. W. Alvarez, F. Asaro, W. Alvarez, and H. V. Michel)

The overall objective of this project is to determine the relationship between asteroidal or other large body impacts on the earth and repeated massive extinctions of life which have occurred in the last 570 million years (m.y.). The primary mechanism for the research consists of intensive chemical and selective mineralogical studies (on sediments near both major and minor extinction boundaries) which are run in parallel with floral and faunal fossil studies by collaborating geologists and paleontologists. A secondary but major objective is to ascertain if a series of time markers of very high precision and accuracy (in the form of iridium and other geochemical anomalies) can be developed for relative dating and correlation of sediments in many different parts of the world. A minor objective is to evaluate the major chemical and mineralogical alterations which have occurred in the sedimentation of the 65 m.y. old Cretaceous-Tertiary boundary, the one most closely linked to a large body impact, in order to predict the behavior expected in older boundaries.

Currently, a new widely distributed iridium horizon and its relationship to impact debris (microtektites) and extinctions are being studied in deep sea sediments 34 m.y. old near the Eocene-Oligocene boundary. Sediments from the Cretaceous-Tertiary (C-T) boundary (65 m.y. old), the Permian-Triassic boundary (∿225 m.y. old), the Frasnian-Famennian boundary (∿350 m.y. old) and the early Cambrian period (∿550 m.y. old) are also being studied.

The correlation between the time of the C-T impact and floral and faunal extinctions which occurred on the continents is being examined in the Western United States and Southwestern Canada.

New techniques for sensitive, rapid and economical measurement of iridium in lithified sediments are being studied to determine the feasibility of a system capable of handling one kilometer of sediment in a few months of measurement time.

L. Fluid Flow in Stressed Rock (P. A. Witherspoon and Y. Tsang)

The objective of this project is to investigate how roughness in a fracture effects fluid flow and to develop the basic understanding of the deformation of the fracture under stress. This work is based on a theoretical model relating mechanical measurements on the rock to fracture geometry at different stress levels. Application of this model permits establishment of a valid fluid flow for a rough fracture over a wide range of stresses. Fluid flow in weathered, filled fractures is also being considered, and a model is being developed to describe this phenomenon under stress changes.

M. Generation and Migration of Petroleum and its Precursor Compounds (O. Weres)

This work reproduces the chemical reactions of petroleum genesis, under conditions which closely resemble those under which petroleum is formed in nature. Emphasis is on the identification of possible water-soluble petroleum precursors. Kerogen-bearing rocks are reacted in an autoclave with brine at high temperature (200-350°C) and pressure, and the organic compounds evolved are separated and identified. Oil and gas field waters are analyzed for organic trace compounds, and laboratory results correlated with field data. The decomposition of water-soluble C-H-O compounds produced in the autoclave experiment will be investigated over a wide range of conditions expected in typical petroleum source beds, except that experimental temperatures will be higher to allow convenient reaction rates.

Contractor: LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California
Livermore, California 94550

Contract: W-7405-ENG-48

Title: I. Geology, Geophysics, and Earth Dynamics

Person in Charge: L. W. Younker

Scope of Work

The Geology, Geophysics, and Earth Dynamics Program at Lawrence Livermore National Laboratory consists of five projects: (A) Thermal and Creep Behavior of Generic Repository Rocks, (B) Diffusion in Silicate Materials, (C) Electrical Conductivity and Temperature in Upper Mantle, (D) Attenuation and Dispersion in Partially Saturated Sedimentary Rocks, and (E) Surface Wave Method for Determining Earthquake Source Mechanisms.

These research tasks are broadly based fundamental studies which have applications in a variety of areas including geothermal energy development, nuclear waste isolation, and seismic verification of nuclear test treaties.

A. Rock Mechanics (H. C. Heard and W. B. Durham)

This laboratory program involves two sub-tasks: 1) determination of the thermal behavior of igneous rocks, and 2) measurement of the creep response of salt.

1. An experiment is being undertaken to measure the thermal diffusivity of igneous rocks to 400°C and 200 MPa lithostatic pressure. For use primarily on rock samples the order of 2.5 cm in diameter, the measurement technique produces precise and accurate measurements in a relatively short time, allowing detailed study to be made of subtle variations of diffusivity with pressure and temperature and of variations from rock to rock. Five different igneous rock types are being measured.

2. This sub-task involves the exploration of the causes responsible for the significant disagreement in the parametric values for the constants in the steady-state flow equation describing the rheological behavior of polycrystalline halite (salt) at moderate temperatures and pressures. The effects of pressure, impurity content, and loading history are being investigated at pressures to 200 MPa and temperatures to 300°C.

B. Diffusion in Silicate Materials (A. J. Piwinskii, F. J. Ryerson, H. C. Weed)

Because oxygen and silicon are major constituents of the earth's crust, the diffusion of oxygen, silicon, and highly-charged cations is being studied over the temperature range of 1000°-1400°C. Compositions vary from almost pure silica (obsidian) to basalt from Halemaumau lava lake, Hawaii. The results of the study should be useful for evaluating the relative magnitude of diffusional and convective transport in geologic systems, and for modeling the thermal evolution of magmas. The results are also applicable to the kinetics of geologically and technologically important processes such as phase separation, crystal nucleation, and crystal growth.

C. Electrical Conductivity and Temperature in Upper Mantle (A. G. Duba) (Joint Project with T. J. Shankland at LANL)

The thermoelectric effect in the mantle minerals olivine and pyroxene is being measured as a function of temperature, orientation, oxygen fugacity, and iron content to investigate the effect of Mg/Si non-stoichiometry on mineral conductivity. The results apply to inference of upper mantle temperatures from electrical data. While there are seismic models to explain the low velocity zone (LVZ) as a solid-state phenomenon not requiring partial melting, the most well-constrained laboratory electrical measurements are more consistent with the partial melting hypothesis for the high conductivity layer (HCL) apparently associated with the LVZ. If the LVZ/HCL is not a partial melt layer, then mantle geotherms would be considerably lower than previously inferred on the basis of a partial melt zone under extensive regions of the earth. Hence, it is necessary to better understand electrical conduction in mantle minerals to find whether electrical data are a serious constraint on the low temperature geotherms suggested by solid state explanations of the LVZ.

D. Attenuation and Dispersion in Partially Saturated Rocks (R. C. Y. Chin, J. G. Berryman, B. P. Bonner, and G. W. Hedstrom)

We will combine theory and experiment to analyze attenuation and dispersion of waves in rocks containing liquid over a broad range of frequencies. The experiments will be carried out on rocks over a broad frequency range using ultrasonics, creep measurements, resonant bars, and impulse propagation. An anelastic long-wave, Pochhammer-Chree theory will be developed. This theory will be used to interpret the experiments, which show both geometric and anelastic dispersive effects. This combined theoretical and experimental approach will yield attenuation and dispersion results at frequencies which are inaccessible to present-day experimental methods. Interpretation and analysis techniques derived from this study will be applicable to a broad range of basic problems in energy recovery, particularly hydrocarbon and geothermal exploration and resource assessment.

E. Surface Wave Method for Determining Earthquake Mechanisms with Applications to Regional Stress Field Studies (H. J. Patton and K. K. Nakanishi)

We will use a method base on surface-wave excitation and seismic moment-tensor theories in order to obtain source mechanisms of remote western United States earthquakes. This method is particularly useful for studying the regional tectonic stress field in areas where there is poor coverage by dense seismic networks, and consequently the P-wave fault-plan solution technique has limited applicability. In the first year of study, we will test our methodology under "controlled" conditions to demonstrate consistency with other stress indicators and magnitude of errors. We will then apply the method to study the state of stress in the northern Basin and Range and its environs. The stress field will be characterized by (1) orientation, using directions of the principal stress axes determined from the focal mechanisms, and (2) magnitude, using the estimate of seismic moment (and field observations, when available) to calculate stress drop or apparent stress. Future work will concern interpretations of the observed stress field in terms of intra-plate sources of stress.

Contractor: LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California
Livermore, California 94550

Contract: W-7405-ENG-48

Title: Geochemistry

Person in Charge: L. W. Younker

Scope of Work

The Geochemistry Program at Lawrence Livermore National Laboratory consists of two projects: (A) Thermodynamic and Transport Properties of Geochemical Systems, and (B) High-Pressure Kerogen Pyrolysis. Studies include laboratory measurements of diffusion coefficients and activity coefficients for mixed salts, and kerogen pyrolysis experiments up to 1kbar. Data obtained in the first task is important for understanding and modeling salt mixtures. The chemical kinetic model for kerogen conversion to petroleum as developed in the second task will have applications in a variety of fossil fuel programs.

A. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions (J. A. Rard and D. G. Miller)

Transport of dissolved chemical species is important in a wide variety of waste isolation and geochemical problems (including diagenesis and ore formation). Mutual diffusion data are needed to understand and model these processes. Osmotic/activity coefficient data are required to understand chemical equilibrium in these solutions (including speciation and solubility). Little diffusion data have been published except for single salts at 25°C, and almost no data are available for salt mixtures or for aqueous systems above 25°C. The situation is somewhat better for activity data, but experimental measurements are required for a wider variety of mixtures. Experimental diffusion and activity measurements, and the development of accurate approximation methods for mixed salts, are essential to fill these large data gaps.

The present task is to measure diffusion coefficients using Rayleigh or Gouy interferometry, and osmotic/activity coefficients using the isopiestic method. Diffusion data are currently being measured for aqueous $MnCl_2$ (ferromanganese nodule formation) and NaCl-$SrCl_2$ mixtures (waste isolation) at 25°C. If time permits, diffusion data will also be measured for NaCl at 50°C and approximation methods tested for estimating mixed salt diffusion coefficients. Isopiestic measurements will be completed for $MnCl_2$ and $MnSO_4$ at 250°C, and measurements started for NaCl-$MgCl_2$ mixtures to their solubility limits.

B. Kinetic and Compositional Model of High-Pressure Kerogen Pyrolysis (A. K. Burnham and J. L. Younker)

The specific goal of this project is to develop a chemical kinetic model for the conversion of kerogen to petroleum along with the associated diagnostic methods necessary to confirm its applicability in a geological setting. To obtain the required data, a series of pyrolysis experiments will be conducted using pressures up to 1 kbar. Pyrolysis products will be analyzed as a function of time to allow characterization of the chemical processes occurring. Time-temperature-pressure histories will be varied sufficiently to provide an improved basis for extrapolation to geological conditions and to develop the diagnostic methods. A detailed chemical model will be derived, and we will explore ways of interfacing chemical and geological models. These models will be valuable as an aid in geochemical exploration and could lead to improvements in extraction techniques for synthetic fuels.

The experimental parameters to be used in assessing the role of alternative reactions in controlling hydrocarbon composition include: organic source material, temperature, pressure, residence time of compounds in reactor vessel, sweep fluids, and mineral species in contact with migrating hydrocarbon phases. This set of parameters is designed to allow consideration of changes in composition of hydrocarbons related to the timing of primary migration, and will provide a better basis for linking the chemical evolution of hydrocarbons to changes in the geological environment.

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Contractor: LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California
Livermore, California 94550

Contract: W-7405-ENG-48

Title: Energy Resource Recognition, Evaluation and Utilization
Continental Scientific Drilling Program: Thermal Regimes

Person in Charge: L. W. Younker

Scope of Work

The Continental Scientific Drilling Program at Lawrence Livermore National Laboratory consists of four projects, (A) Data Management, (B) Underground Imaging, (C) Viscosity Measurements, and (D) Thermal and Petrologic Studies of Silicic Systems. These projects support the overall program in a variety of ways, including information and data management service, generic studies on site characterization techniques, generic studies on laboratory measurements of melt properties, and studies of fossil analogue systems.

A. Continental Scientific Drilling Program Information and Data Management Unit (N. W. Howard)

Because of the extremely high cost of drilling, it is crucial that the geologic community be kept informed of the availability of drill holes and the data obtained from them. Numerous governmental agencies and research groups have drilled holes for a variety of purposes. In some cases, information has been disseminated on the availability of these holes for research purposes and cooperative programs have been initiated between a number of academic, government, and industrial groups. More often, however, this information has not been disseminated and interested researchers have been unaware of the availability of these drill holes until it is too late to participate effectively. An information system has been established to avoid this problem. The efforts of a continental scientific drilling program (CSDP) can be expedited, unnecessary expenditures limited, and maximum data effectiveness attained, by utilization of pre-existing information; (2) reopening of abandoned holes; (3) participation in current industry drilling tests; and (4) participation in the drilling and study of future wells.

LLNL has developed a computerized data base for drill hole data acquired in CSDP projects, and is providing information to the scientific community on plans and drilling activities in a timely manner. It will continue to do so through the initial period of intensive use. A study of potential long-term operating modes has proved that there is still an active interest in the data base which is best served by having LLNL provide data compilations as requested by researchers.

B. Underground Imaging (A. G. Duba and R. J. Lytle)

A significant portion of the Department of Energy budget is being spent on extracting energy from, or storing nuclear waste within, the subsurface environment. To assess whether the energy extraction or waste storage procedures are properly implemented, it is necessary to obtain detailed images of the subsurface environment. Such images will also be of value for continental drilling interests. LLNL has had success in developing and applying the concept of geophysical tomography to achieve such images. LLNL has also shown that improved interpretations of the subsurface environment can be obtained by combining laboratory data on the relations between remote probing observables (such as seismic attenuation or electromagnetic velocity) and the governing physical phenomena (such as in situ stress or temperature). This effort will continue the integrated program for advancing the state-of-art in data collection methods, data processing procedures, data interpretation techniques, and enhanced means of data interpretation. This coordinated program involves a cooperative effort by LLNL and university researchers to achieve a balanced perspective. This balance requires efforts in fundamental studies, instrument development, data processing, data integration and interpretation, and field demonstrations.

C. Viscosity and Electrical Conductivity of Rock Melts: Continental Scientific Drilling Program (A. J. Piwinskii, F. J. Ryerson, and H. C. Weed)

In order to understand the transport of mass and energy in geological processes, we are determining viscosities and electrical conductivities for molten silicate systems. These include basalt from Kilauea Iki lava lake, Hawaii, and compositions corresponding to targets selected for deep continental drilling. The results should help clarify relationships between melt composition and viscosity, to model the evolution of magmatic systems, and to establish a correlation between transport and other properties for molten silicates.

D. Thermal and Petrologic Studies of Large Silicic Systems [L. W. Younker, P. W. Kasameyer, and T. A. Vogel (Michigan State University)]

Integration of petrologic studies and the thermal studies will eventually lead to an overall improved understanding of shallow silicic systems, and provide the basis for the development of predictive models which can be tested by deep drilling at a young system.

Petrologic Studies: We have identified three field sites which can contribute to the basic understanding of the petrologic evolution of silicic systems.

- o Acidic-Basic complex of Ardnamurchan in Scotland.
- o Black Mountain caldera in Nevada.
- o Elkhorn Mountains/Boulder batholith complex in Montana.

Petrologic studies of these three systems are presently underway. Synthesis of the results of these studies will shed light on characteristics of both large-volume and small-volume silicic systems. These systems have been selected because they add critical information to augment the existing petrological models.

Thermal Studies: We are working to improve the present generation thermal models of shallow magma systems. Contact metamorphic aureoles provide a record of heat transfer mechanisms within and around shallowly emplaced igneous intrusions. We have used information from several exposed systems to constrain heat transfer mechanisms. This information will be used in conjunction with other constraints to improve the thermal modeling capabilities.

E. CSDP: Imperial Valley Information Base (D. O. Emerson and P. W. Kasameyer)

An integrated information base containing references to published geologic, geophysical and geochemical data and interpretations is essential in considering detailed site selection for CSDP-Thermal Regimes. The information base will contain:

(1) Bibliographic information in standard reference format with keyword-based identification of data presented in the reference.

(2) A listing of researchers who are currently engaged in active research in this area, with a brief statement of type, nature, extent, and objectives of the research.

(3) Brief summary of generalized plans for future research, including shallow, intermediate and deep drilling.

The Information Base will be prepared on a stand-alone microcomputer using a conventional commercial data base management system. Information will be distributed in printed form on a semi-annual basis.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: I. Geophysics

Person in Charge: J. T. Whetten

Scope of Work

Geophysics research at Los Alamos National Laboratory presently consists of four subtasks: (A) Creep deformation of Rock; (B) Radiative Heat Transfer in Minerals, Glasses and Melts; (C) Electrical Conductivity and Temperature in the Upper Mantle; and (D) Nonlinear Generation of Acoustic Beams.

(A) Creep deformation of basalt, granite, and tuff is studied at simulated in situ conditions of temperature, pressure, pore pressure, and differential stress. Emphasis is placed on evaluating effects of water on time-dependent brittle deformation of intact vs. fractured samples. Results of the experiments are formulated into creep constitutive relations in a form amenable to predictive computer models.

(B) The contribution to total thermal conductivity from the radiative component is determined in a variety of minerals important in geothermal and waste isolation research. Radiative thermal conductivity is calculated as a function of temperature from measured optical absorption spectra taken at exceptionally high temperatures to 1500°C in a controlled atmosphere.

(C) The thermoelectric effect in the mantle minerals olivine and pyroxene is measured as a function of temperatures, orientation, oxygen fugacity, and iron content. The effect of Mg/Si nonstoichiometry on mineral conductivity is investigated. The results apply to inference of upper mantle temperatures from electrical data.

(D) The interactions of two high-frequency-sound beams are measured in fine-grained, dense rocks to determine the nonlinear acoustic properties of rock. If narrow-beam, difference-frequency sound can be propagated, numerous applications to problems in exploration geophysics, in situ monitoring, and rock property investigations are possible.

These research tasks apply importantly to technology needs in waste isolation and geothermal energy.

A. Creep Deformation of Rocks (J. D. Blacic)

Assurance of long-term isolation of nuclear wastes in mined cavities in hard rock requires knowledge of time-dependent strength and transport properties of these rocks. Normal, short-time engineering tests do not encompass the full effects of phenomena such as water-aided stress corrosion and hydrolytic weakening. Therefore, we study creep deformation of basalt granite and tuff at simulated in situ conditions of temperature, pressure, pore pressure, and differential stress. Emphasis is placed on evaluating effects of water on time-dependent brittle deformation of intact vs. fractured samples and its effect on fluid permeability. Results of the experiments will be formulated into creep constitutive relations in a form amenable to predictive computer models of repository designs.

B. Radiative Heat Transfer in Minerals, Glasses, and Melts (T. J. Shankland)

We are determining the contribution to total thermal conductivity from radiative heat transport in a variety of materials that figure in geothermal studies and nuclear waste isolation. We can calculate radiative thermal conductivity as a function of temperature from measured optical absorption spectra taken at exceptionally high temperatures, up to 1500°C, in a controlled atmosphere.

Heat transport is at the center of many geophysical problems. Our measurements of radiative heat conductivity K_R in magmatic glasses indicate that this is a surprisingly large heat transfer mechanism in crustal magma chambers, and we are extending the measurements to actual melts. Another application of the same apparatus is to heat transfer in glasses used for nuclear waste isolation. Finally, we plan to continue work on K_R of crystalline materials.

C. Electrical Conductivity and Temperature in the Upper Mantle
[T. J. Shankland and A. G. Duba (Lawrence Livermore National Laboratory)]

We are measuring thermoelectric effect in the mantle minerals olivine and pyroxene as a function of temperature, orientation, oxygen fugacity, and iron content and are investigating the effect of Mg/Si nonstoichiometry on mineral conductivity. The results apply to inference of upper mantle temperatures from electrical data. While there are seismic models to explain the low velocity zone (LVZ) as a solid-state phenomenon not requiring partial melting, the most well-constrained laboratory electrical measurements are more consistent with the partial melting hypothesis for the high conductivity layer (HCL) apparently associated with the LVZ. If the LVZ/HCL is not a partial melt layer, then mantle geotherms would be considerably lower than previously inferred on the basis of a partial melt zone under extensive regions of the earth. Hence, it is necessary to better understand electrical conduction in mantle minerals to find whether electrical data are a serious constraint on the low temperature geotherms suggested by solid state explanations of the LVZ.

Because temperature differences drive tectonic motions on the earth's surface and interior, improved knowledge of thermal patterns is a requirement for evaluating seismic and volcanic hazards to waste isolation and power plant sites. Further locating high temperatures is an essential for regional geothermal prospecting, particularly for the Los Alamos Hot Dry Rock project. The results should clarify our understanding of the regional geophysics needed for continental drilling site selection and for nuclear event detection and discrimination.

D. Nonlinear Generation of Acoustic Beams (T. J. Shankland and J. N. Albright)

We are using the nonlinear elastic properties of rocks to generate low frequency, long-wavelength acoustic beams in analogy with the case in laser optics. Two narrow beams of high-frequency sound can interact in a nonlinear medium to produce a narrow beam at their much lower difference frequency. The lower frequency beam has the narrow width of the generating beams, but it can travel much farther because of lower attenuation. Such a narrow beam would permit examination of acoustic interfaces from mine interiors and wellbores without the ambiguities of conventional seismology that uses undirected sources, for example, transducers or explosives that broadcast energy in an almost spherical pattern. Should beam formation prove possible, there would be numerous applications to problems such as mapping fractures, the boundaries of ore and coal bodies, burn fronts in underground retorts, and fluid locations in oil, gas, and geothermal reservoirs. Of more interest to basic research in rock physics is the investigation of nonlinear properties of rocks and frequency dependence of elastic properties.

Nonlinear acoustic beams have previously been observed in homogeneous materials and fluids; however, rocks have the advantage of much greater nonlinear coefficients owing to the strong effect of crack closure on elastic properties. In preliminary results we have observed difference frequency generation from Vibroseis transducers operating in the field and from piezoelectric transducers on laboratory specimens at high frequencies.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: II. Geochemistry

Person in Charge: R. W. Charles

Scope of Work

Research in geochemistry consists of seven subtasks: (A) Rock-Water Interactions, (B) Element Migration and Fixation in Rocks, (C) Physiochemical Basis of the NA-K-Ca Geothermometer, (D) Cation Site Size and Coulomb Energy Calculations for the Principal Rock-Forming Minerals, (E) Coal Maturation: Occurrence, Form, and Distribution of Sulfur and Mineral Matter in Peat, (F) Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures, and (G) Geochemistry of Technetium and Ruthenium and Geochemical Controls on the Redistribution of Multivalent Elements in the Lithosphere.

(A) Rock-water Interactions deals with hydrothermal experiments and theoretical calculations which model reactions in rock reservoirs using static, agitated, and dynamic (circulatory) systems. Theoretical approaches involve detailed chemographic relations and mass transport theory.

(B) Element Migration and Fixation in Rocks studies the location, mobilization, and deposition of trace elements in various rock reservoirs.

(C) The Physiochemical Basis of the Na-K-Ca Geothermometer seeks to define the phase equilibria underlying the Na, K, and Ca composition in solutions and will attempt to widen the geothermometer's usefulness.

(D) Cation Site Size and Coulomb Energy Calculations will contribute to the understanding of inter- and intracrystalline major and trace element fractionation trends and help define the effects of some accessory phases on whole-rock trace element distributions.

(E) Coal Maturation: Occurrence, Form, and Distribution of Sulfur and Mineral Matter in Peat will determine the botanical and depositional environment controlling the mineral matter found in peat, the precursor of coal.

(F) The Thermodynamic Properties of Aqueous Solutions of High Temperatures and Pressures studies the properties at aqueous electrolyte solutions by flow calorimetry.

(G) The Geochemistry of Technetium and Ruthenium and Geochemical Controls on the Redistribution of Multivalent Elements in the Lithosphere examines the mobility of these elements in nature in order to assess the effectiveness of potential geologic sites for nuclear waste repositories.

A. Rock Water Interaction in Geothermal Systems (R. W. Charles, T. M. Benjamin, and G. K. Bayhurst)

Rock and fluid are equilibrated in various hydrothermal systems in order to model reactions of interest to the Department of Energy concerning a number of rock reservoirs. Experimentation can involve reaction in static (cold seal), agitated (Dickson vessel), or dynamic (circulation) systems. The most advanced circulation system, constructed of titanium can examine reactions with chloride solutions in a temperature gradient. Maximum conditions are 350°C and one kilobar pressure for durations of up to nine months. Rock reactions and solution compositions are continually monitored by SEM and plasma emission spectroscopy, respectively.

The observed alteration assemblages are related in a chemographic network of suitable intensive variables (pressure, temperature, and chemical potentials) characteristic of the experiment. The chemographic results yield assemblages not directly observed in the experiment. The results allow one to postulate the results of longer duration experiments done under slightly different physical constraints and how these affect the rock reservoir with time.

B. Element Migration and Fixation in Crustal Rocks (T. M. Benjamin, P. Z. Rogers, and R. W. Charles)

Rocks and pure minerals are reacted with solution in order to learn more about the behavior of trace elements, some of which are of economic value. The questions asked are (1) Where is the element located in the crystal lattice?, (2) How is this element mobilized?, (3) What speciation is involved in transport?, and (4) How is the element precipitated? Experiments are conducted in agitated (Dickson vessels) and dynamic (circulation) systems. Solid phases are analyzed by proton microprobe, electron microprobe, and scanning electron microscope. Solutions are analyzed by ion chromatography and plasma emission spectrometry.

These studies can examine and help alleviate some of the cost of geothermal energy extraction, examine the origin of ore bodies, and examine the behavior of elements in a hazardous waste repository.

C. Physiochemical Basis of the Na-K-Ca Geothermometer (R. W. Charles, T. M. Benjamin, and G. K. Bayhurst)

The Na-K-Ca geothermometer was developed empirically by R. Fournier and A. Truesdell (USGS) to determine the temperatures of a rock reservoir at depth simply from the amount of Na, K, and Ca found in the fluid as it emerges at the surface. It has undergone some modification in succeeding years to take into account other elements in the solution. Direct application of the geothermometer occurs in, particularly, geothermal reservoirs. The usefulness of this technique is limited because its chemical basis is not understood. A series of experiments is under way to determine what phases control the Na, K, and Ca concentrations in solution. The activities of these elements are fixed by secondary phases produced by reaction of the feldspars (+ quartz) with water as the rock and water move toward mosaic equilibrium. The discovery, composition, and structure of these overgrowths is the thrust of the experimentation. Because many of the geothermal systems emanate from granite-like rock, granite plus aqueous solution is being examined closely in static (cold seal vessels), agitated (Dickson vessels), and dynamic (circulation) systems.

D. Cation Site Size and Coulomb Energy Calculations for the Principal Rock-Forming Minerals (D. L. Bish, J. R. Smyth)

Calculations are underway to determine mean bond distances, volumes and distortion indices for coordination polyhedra, and coulomb potentials for all cation and anion sites using published crystallographic data for ordered end-members of the common rock-forming minerals. These calculations, together with some modeling of crystal structures, will improve our understanding of inter- and intracrystalline major and trace element fractionation trends. These data, not presently available, will enable us to predict the effects of accessory phases on whole-rock trace-element distributions, and the data will have wide application in predicting the distribution of minor and natural trace elements in natural and man-made materials.

We have completed calculations for the anhydrous rock-forming minerals and are beginning to work on hydrous minerals. This work will be aimed particularly at understanding and predicting the distributions of hydroxyl, fluoride, and chloride ions between minerals. Results of our calculations will be collected in a reference publication.

E. Coal Research: Occurrence, Form and Distribution of Sulfur in Peat (R. Raymond, Jr., A. D. Cohen, and R. Gooley)

Elemental, mineralogic, and petrographic compositions of peats, the precursors of coals, are controlled by a combination of botanical and depositional environments. Diagenic alterations occur within these various environments that will eventually affect the occurrence of sulfur and/or mineral matter in a coal deposit; one must understand the mechanisms for their introduction into the original peat deposit and the alterations they go through during stages of peatification.

We are investigating sulfur and mineral matter emplacement, distribution, and alteration in three distinct coal-forming regions: marine to brackish water environments (Everglades, SW Florida); salt marsh/freshwater complex (Snuggedy Swamp, South Carolina); and freshwater swamp-marsh complex (Okefenokee Swamp, Georgia). The objectives of our research are: (1) to identify and correlate sulfur forms, authigenic minerals, and detrital minerals found in different peat types; (2) to identify the processes that enhance and/or inhibit distribution and preservation of sulfur and mineral matter in the initial coal forming environment; and (3) to construct geochemical models for their formation, preservation, alteration, and distribution based on the first two objectives.

Our approach is to use electron probe microanalysis, scanning electron microscopy, bulk chemical analyses, and conventional sedimentological analyses to characterize the models of occurrence and content of both sulfur forms and biogenically and non-biogenically derived mineral matter in peat types. We will thereby be able to establish the relationship between sulfur and mineral matter occurrence and peak types, and also to correlate the concentration and forms of their occurrence with specific environments of deposition.

F. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures (P. Z. Rogers, T. M. Benjamin, R. W. Charles)

Knowledge of the thermodynamic properties of aqueous solutions is basic to an understanding of many geochemical systems. Hydrothermal alteration, element migration, geothermal activity, and integrity of waste repositories are a few examples of processes largely dependent on the properties of the associated aqueous fluid. Studies of these processes require information on the heat content and ion activities of mixed electrolyte solutions over a wide range of composition and temperature.

A flow calorimeter has been designed to measure the heat capacities of single and mixed electrolyte solutions over a temperature range from 25°C to 350°C and at pressures from saturation to 500 bar. The heat capacity data can be integrated as a function of temperature to determine solution enthalpies and the ion activities of solution species. These thermodynamic properties will be used to provide an accurate model for electrolyte solutions at high temperatures and pressures.

G. Geochemistry of Technetium and Geochemical Controls on the Redistribution of Multivalent Elements in the Lithosphere (D. B. Curtis, R. Perrin, and D. Rokop)

An understanding of the long-term stability of ^{99}Tc in a geologic environment is critical to evaluating the effectiveness of geologic sites for the disposal of nuclear wastes. Technetium exists in nature only as a fission product of the spontaneous fission of ^{238}U. This quantity is extremely small, below the detection limit of most analytical methods, and thus there have been no direct observations concerning the geochemistry of technetium. Nuclear waste site evaluations with regard to this element must be based upon inferences from laboratory and theoretical work.

The spontaneous fission product ^{99}Tc has a half life of $\sim 2.13 \times 10^5$ years. Because both the parent, ^{238}U, and the daughter are radioactive, in a closed chemical system these two nuclides establish a state of secular radioactive equilibrium. In such a state, the atomic ratio of the two elements is a well defined constant. Technetium-99 decays to the stable nuclide ^{99}Ru. This is one of four ruthenium isotopes produced by radioactive fission. The other three are produced instantaneously, while the rate of production of ^{99}Ru is slowed because of intervention of the long-lived precursor ^{99}Tc. In a closed chemical system the isotopic composition of spontaneous fission product ruthenium is fixed. In a system where ruthenium has been fractionated from technetium, the isotopic composition of ruthenium will be altered showing either an excess or deficiency of ^{99}Ru.

Measurements of the abundance of uranium, ^{99}Tc and the isotopes of ruthenium provide the means to evaluate the relative geologic stability of uranium and ^{99}Tc in recent times, and ruthenium, technetium and uranium during the period of time since the host rock was formed. We have developed procedures to measure ^{99}Tc and the isotopic composition of ruthenium in uranium-rich rocks by isotope dilution mass spectrometry. The methods will be applied to examine the geochemistry of these elements.

Previous work has demonstrated unexpected movement of technetium during the period of nuclear criticality of the natural fission reactors found in the Oklo mine in Gabon, Africa. We will measure ^{99}Tc abundances in rocks to determine the stability of the element in recent times. Samples for the analyses have been selected for these measurements and uranium abundances have been determined.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: Thermal Regimes and Continental Scientific Drilling Program

Person in Charge: J. T. Whetten

Scope of Work

Research in Thermal Regimes and the Continental Scientific Drilling Program at Los Alamos National Laboratory consists of four items: (A) Studies of the Polvadera Group, (B) Origin and Extent of the Toledo Caldera, (C) Anomalous Lithospheric Structure Beneath Valles Caldera, and (D) Valles Caldera Information Base.

(A) The Polvadera Group of the Jemez Mountains is studied to determine its overall composition, the origin of its magmas, timing of eruptions, sequences of compositional variation, and its relations to older and younger volcanic units. The work is directed toward understanding the evolution of the magma chamber(s) beneath the Jemez Mountains.

(B) The location and extent of the buried portion of the Toledo caldera in the Jemez Mountains is to be determined. Geochronology, stratigraphy, and petrology of domes and volcanic and sedimentary deposits in the exposed part of the caldera will be studied.

(C) Teleseismic short-period P-wave delays and synthetic seismogram modeling of crustal transfer functions will be used to delineate regions of anomalous seismic wave propagation and attenuation beneath the Jemez Mountains (including Valles caldera).

(D) An information data base is being established for CSDP thermal regime studies of the Valles caldera.

A. Field, Petrologic and Geochemical Studies of the Polvadera Group, Jemez Mountains, New Mexico (W. S. Baldridge and D. T. Vaniman)

The Jemez Mountains of northern New Mexico are a major basaltic-to-silicic, late Cenozoic volcanic field, lying at the intersection of the Jemez lineament and the Rio Grande rift. Volcanism in the Jemez Mountains began 12-13 m.y. ago. Caldera formation occurred 1.4 and again 1.1 m.y. ago with the eruption of the major ash flow sheets, followed by caldera collapse, resurgent domes, and additional small ash flows. The Jemez Mountains volcanic field is presently the focus of intense research interest for these reasons: (1) The Jemez Mountains are a major source of our information for understanding caldera formation, ash flow emplacement, and magma resurgence. (2) Data from the Jemez Mountains have contributed to what little is known about the complex magmatic evolution processes associated with high-level silicic magma chambers. (3) The Jemez Mountains are a focus of major hydrothermal activity and high heat flow.

The Polvadera Group (Tschicoma and Lobato Formations) northeast of Valles caldera is being studied to determine its overall composition, the origin of its magmas, the timing of eruptions, sequences of compositional variation, and the relationship to older and younger volcanic rocks. This project will be directed to understanding the magma chamber(s) that were active 2-10 m.y. ago, of factors governing changes in magma composition, and of the overall history of the Jemez Mountains.

B. Origin and Extent of the Toledo Caldera, Jemez Mountains, New Mexico, and its Relation to the Valles Caldera (G. H. Heiken and F. E. Goff)

The Toledo caldera is the older of two large calderas in the Jemez Mountains formed during the eruption of upper and lower members of the Bandelier Tuff. The location and extent of the Toledo caldera is not well understood because most of the caldera has been masked by the younger Valles caldera. If a borehole is drilled by the Continental Scientific Drilling Program within the Valles caldera, one objective would be to choose a drill site located within the overlap of the Toledo and Valles calderas in order to gain maximum information on the history of the calderas and their geothermal systems. The principal objective of the project is to locate the area of overlap of the two calderas. We propose to do this through geochronologic, stratigraphic and petrologic study of the domes, and pyroclastic and sedimentary deposits located within the exposed remnant of the Toledo caldera. These data should provide information on source areas for these deposits within the Toledo caldera and, indirectly, its original location and extent.

C. Anomalous Lithospheric and Asthenospheric Structure Beneath the Valles Caldera/Rio Grande Rift of New Mexico (K. H. Olsen)

This project is to investigate lateral variations in crustal and uppermost mantle structure and the relationship of these variations to the major volcano-tectonic geothermal regimes of northern New Mexico. Specifically, we are using the techniques of (1) teleseismic short-period P-wave delays, together with (2) synthetic seismogram modeling of crustal transfer functions, to define the regions of anomalous seismic wave propagation and attenuation beneath the Jemez mountain volcanic field, which is one of the principal components of the Rio Grande Rift system of Colorado, New Mexico, Texas, and Mexico.

Our previous seismic studies in northern New Mexico have mainly used seismic waves from local and regional earthquakes and from available explosions to "illuminate" local structures from the side. CARDEX 81, for example, was the field-recording phase of a series of crustal refraction and fan shooting profiles in the Jemez Mountains/Rio Grande rift. The analysis and interpretation of this large data set continues and will be merged with future data to provide constraints in interpretation of future experiments. In contrast, the CARDEX 83 experiment will concentrate on "illuminating" structures from below, using seismic waves at nearly vertical incidence angles from distant (greater than 3000 km) earthquake sources. The data will complement those from previous studies, and the region of principal focus will shift from the shallow crust (depths less than 20 km) to the deeper crust and the uppermost mantle within approximately 50 km of the Moho.

D. Valles Caldera Information Base (N. L. Marusak and F. Goff)

An integrated information base containing references to published geologic, geophysical and geochemical data and interpretations is essential in considering detailed site selection for CSDP-Thermal Regimes. We will establish an information base that will contain (1) bibliographic information in standard reference format with Keyword-based identification of data presented in the reference; (2) a listing of researchers who are currently engaged in active research in this area, with a brief statement of type, nature, extent, and objectives of the research; and (3) a brief summary of generalized plans for future research, including shallow, intermediate, and deep drilling.

The Information Base will be prepared on a stand-alone microcomputer using a conventional commercial data base management system. This computer system will be Inter-Lab compatible and accessible. The formatting of Valles Caldera Information Base will be consistent with the Long Valley and Salton Sea Information Bases. Information will be distributed in printed form on a semi-annual basis.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: IV. Space Plasma Physics

Person in Charge: D. N. Baker

Scope of Work

The objective of this program is to analyze and interpret existing satellite data from the solar wind and earth's magnetosphere to yield an understanding of physical mechanisms and long-term effects of sun-earth coupling through the solar wind and to understand sources of free energy in these plasma particle velocity distributions. Since the solar wind and magnetospheric plasmas are the media through which solar-generated disturbances propagate and in which solar wind convection energy is stored and subsequently released to the auroral ionospheres, these studies help us understand the coupling of solar variations to the near-earth environment. This research relates to the Department of Energy's missions through applications to plasma physics and magnetohydrodynamics (MHD) problems relevant to fusion energy technology, understanding long-term solar wind and earth climate variability, and future space-based energy technologies.

A. Energy Transport in Space Plasmas (S. P. Gary and W. C. Feldman)

The long-term goals of this research are to describe the structure of and flow of plasma energy in the solar wind and the earth's bow shock, magnetosphere and ionosphere. Specific aims include determining the properties of the electron and ion distribution functions in the solar wind in order to better understand heating and transport processes, and understanding solar wind-magnetosphere coupling through fundamental studies of plasma instabilities and transport in and near the earth's bow shock, magnetosphere and ionosphere.

Our most important research result in 1982 came from a joint experimental and theoretical analysis of electron distributions within the earth's bow shock. Our data analysis, using data from high time resolution plasma analyzers on the ISEE spacecraft, demonstrated for the first time the existence of an electron beam aligned parallel to the magnetic field within the bow shock. Our theoretical analysis modeled such electron distribution functions and showed that they can generate an ion acoustic instability with properties similar to those observed for fluctuations within the shock. Since most previous theories of current-driven microinstabilities within the shock have concentrated on models driven by currents perpendicular to the magnetic field, our results offer a new approach to the study of wave-particle transport in collisionless shocks.

B. Electrodynamical Aspects of the Solar Wind-Magnetosphere Interactions (E. W. Hones, Jr.)

The interaction of the solar wind with the earth's magnetosphere is essentially electrical in character, very much resembling the working of a magnetohydrodynamic (MHD) electrical generator. Solar wind plasma, impinging on the earth's magnetic field, flows through its outer regions (the "boundary layer" and gives up its energy to the generator of electrical currents that flow into the ionosphere, depositing energy there. Currents also flow across and around the tail, creating the tail lobe magnetic field, a storehouse of magnetic energy that is drained away both continuously and intermittently during substorms. Much of the intermittent loss during substorms involves severance near the earth of a portion of the plasma sheet, forming a plasmoid which then drifts out of the tail and is lost.

We use data from satellites in the outer magnetosphere to seek quantitative understanding of at least some of the elements of this global system of energy exchange and conversion. Some important results of our research in the past year are:

(1) Further identification of plasmoids and their association with substorms.

(2) Further determinations of the properties of plasma vortices, the very large scale ($\sim$5 to 30 R_E) patterns of rotating plasma flow that drift tailward through the plasma sheet and that may be generated by an instability in the boundary layer.

C. Theory of Energetic Electron Acceleration and Precipitation from the Terrestrial Magnetosphere (D. N. Baker)

In this research effort we address the details of fundamental acceleration processes and resonant wave-particle interactions in the earth's outer radiation zone. These aspects of energetic particle studies deal specifically with the problem of how energetic electrons are generated and subsequently lost from the magnetosphere into the auroral ionosphere. Our initial approach is to study the loss of energetic electrons from the terrestrial magnetosphere. This work is done within the general framework of the Kennel-Petschek theory, with new features that we develop using a strong interplay between analytic and computer calculations in both linear and nonlinear theories. We test these results against the excellent Los Alamos particle measurements being made at geostationary orbit, and we compare available wave data with particle observations and theoretical estimates of wave energy densities. Our studies in this area bear on several problems of interest to DOE. Specifically, they bear strongly on (1) understanding plasma acceleration processes such as accompany the production of fusion plasmas, (2) understanding the relationship between plasma microinstabilities and the imperfect confinement of hot fusion plasma particles, (3) understanding the coupling between the terrestrial magnetosphere and troposphere (which possibly affects climate variability), and (4) assessing the hazards and economic viability of the near-earth environment with regard to space-based human activity (e.g., future energy generation and transmission technologies).

40-574 O - 85 - 38

Contractor: OAK RIDGE NATIONAL LABORATORY
Union Carbide Corporation
Oak Ridge, Tennessee 37830

Contract: W-7405-eng-26

Title: Geochemistry of Crustal Processes at High Temperatures and Pressures

Person in Charge: R. E. Mesmer

Scope of Work

This program provides basic geochemical information on hydrothermal and magmatic processes involving both homogeneous and heterogeneous systems emphasizing the high temperature and high pressure regimes that promote transport and redistribution of materials in the crust. Special facilities are employed in experimental studies including a hydrogen service, internally heated vessel for studies to 1400°C and 500 MPa. Dickson type apparatus and emf cells, conductance, calorimetric and isopiestic facilities are utilized in hydrothermal work to conduct speciation, equilibrium and kinetics studies on selected model systems. Detailed thermodynamic and kinetic information on well chosen specific systems is needed to provide the data base for the quantitative modeling of the complex mixtures in natural rocks and fluids. The important geochemical questions addressed are magmatic and volcanic processes, element cycling, rock evolution and alteration, ore deposition, and the geochemical consequences of waste storage and extraction of geothermal energy.

Present research has provided information on phase equilibria, crystallization kinetics, redox reactions, chemical fractionation and element fractionation in certain magmatic systems. In hydrothermal systems speciation and equilibrium studies have been conducted on water, aqueous carbon dioxide, silicic acid, fluorosilicates, calcium and magnesium ions, and tungsten as well as solubility data on amorphous SiO_2 and quartz.

A. Silicate Melt Geochemistry

Olivine Nucleation and Growth Kinetics in Synthetic Basalt Magmas (M. T. Naney)

Crystal nucleation and growth experiments are conducted at 100 kPa to investigate nucleation delay and the crystal growth rate of olivine (Mg_2SiO_4) precipitating from two Fe-free model basaltic liquids. This study will provide data concerning: (1) the influence of viscosity on crystal nucleation, (2) initial olivine growth rates that may be compared with "average" growth reported for olivine in the literature, and (3) the influence of nucleation delay phenomena on growth rate values as calculated from isothermal crystallization experimental data.

Crystal nucleation and growth rate data to be obtained in this study are needed for the development of quantitative models of basaltic magma flow and consolidation.

Iron Redox Equilibrium Kinetics in Silicate Liquids (M. T. Naney, S. E. Swanson, Univ. of Alaska)

Controlled atmosphere experiments are conducted at 100 kPa to investigate iron redox reactions in silicate melts. Studies in progress are designed to test assumptions about the kinetics of these reactions made in recently published reports. We believe that assumptions about redox kinetics made by others have been too optimistic, with regard to silica-rich compositions. An important consequence of underestimating the time required for silicate melts to reach redox equilibrium is that ferrous-ferric iron ratios obtained from such samples would be non-equilibrium values. We believe that non-equilibrium data has been used to formulate functional relationships to calculate equilibrium oxygen fugacity of magmas in terms of temperature, bulk composition, and Fe^{+2}/Fe^{+3} ratios.

A series of timed experiments with each of three silicate liquids derived by melting natural volcanic rocks of widely varying composition (basalt, andesite and rhyolite) will be conducted at 1243°C and two redox conditions: log f_{O_2} = -6.05 and -7.83, (quartz-fayalite-magnetite buffer) in a CO/CO_2 gas mixing vertical tube-furnace. Additional studies of silicic calc-alkaline melts, using the previously obtained kinetic data, will be conducted to investigate the influence of redox conditions on crystallization. The goal of these studies is to understand the influence of redox conditions on chemical fractionation and crystallization of magmas in the crust.

Stability of "Magmatic" Epidote in Granitic Rock Systems (M. T. Naney)

The recently installed hydrogen-service internally heated pressure vessel will be used to investigate the stability of epidote [$Ca_2(Al,Fe)_3Si_3O_{12}(OH)$], a common accessory mineral of silicic plutonic rocks. Experiments will be conducted to define the coexistence of epidote with hydrous granitic melts as a function of temperature (500-700°C), pressure (200-800 MPa), bulk composition, and oxygen fugacity. A pressure dependence for this coexistence has been demonstrated (Naney, in press) that may provide a single point "geobarometer" under favorable geologic conditions. This study will quantify the pressure dependence of epidote-melt coexistence in granitic systems and provide phase stability data that will be needed in a subsequent study of uranium and thorium chemical partitioning among coexisting silicic liquids, aqueous vapor, and crystalline phases.

B. Hydrothermal Geochemistry

Magnesium Hydrolysis and Brucite Solubility in High Temperature Aqueous Sodium Chloride Solutions (S. E. Drummond)

Recent estimates of the ΔH of the first hydrolysis step for magnesium (14.9 kcal/mole, Baes and Mesmer) along with the value of the equilibrium constant (K_1) at 25°C ($\sim 10^{2.3}$) corresponds to an estimated value for K_1 of $10^{7.7}$ at 300°C. This evidence indicates that magnesium is largely hydrolyzed in near neutral solutions at high temperature and suggests that about 10^{-4}m OH^- is freed when a neutral solution with 10^{-3}m total magnesium is cooled from 300° to 200°C. Consequently magnesium may play a more important role in influencing the pH of natural hydrothermal solutions than previously realized. The exact nature of this effect depends on the interaction of magnesium with OH^- and with other anions such as chloride at high temperature. Ongoing experiments on the hydrolysis of magnesium and the solubility of brucite [$(MgOH)_2$] in sodium chloride solutions will establish the role of magnesium in hydrothermal solutions.

Kinetics of the Thermal Decarboxylation of Acetate and the Role of Catalysis (S. E. Drummond, D. A. Palmer, F. W. Dickson)

This research is focused on the hypothesis that natural gas migrates as acetate from the source in a sedimentary basin and that the acetate decomposes at or near the reservoir to CH_4 and CO_2. The idea is attractive because acetate, unlike CH_4, is completely miscible in water and consequently is more mobile in water-laden sediments. The hypothesis is plausible if the time required to decompose acetate is compatible with the fluid migration time from source to reservoir. In order to address this point, experiments on the effects of temperature, composition, and catalysis on the thermal decomposition rates of acetate are in progress.

Hydrothermal Transportation and Deposition of Tin, Tungsten and Molybdenum (S. E. Drummond and D. Wesolowski)

Hydrothermal tungsten ores are commonly associated with relatively high concentrations of either tin or molybdenum but rarely both. Tungsten and molybdenum are usually associated in relatively oxidized porphyry systems whereas the tin-tungsten association is most common in reduced environments. Recent experimental work has shown that tungsten is transported in the +6 state as HWO_4^-, even in extremely reducing conditions. These observations suggest that, like tungsten, molybdenum is transported in the +6 state but over a more limited range of f_{O_2}. Tin, however, is probably mobile only in the +2 valence state and only is reduced systems. Experimental studies of the hydrolysis of tin and molybdenum and the solubilities of cassiterite (SnO_2), powellite ($CaWO_4$) and molybdenite (MoS_2) are planned in order to test this hypothesis and quantitatively evaluate the mineralization processes associated with granitoids.

Reaction of Silica Phases with Aqueous Solutions (F. W. Dickson)

Scientific studies on the shallow earth's crust and practical uses as well commonly need data on modes of interaction of the common silica minerals (quartz and amorphous silica) with aqueous solutions that range from dilute, recently injected, meteoric waters to concentrated brines. Crustal processes from 20°C to 300°C and 0.1 to 50 MPa follow reaction paths that may depart substantially from equilibrium, which requires detailed knowledge of kinetic steps as well as the equilibria among the involved phases. The reactions of quartz, and to a lesser degree of amorphous silica, with H_2O, $NaNO_3$ solutions, NaCl solutions and buffered NaCl solutions are being determined at temperatures in the interval 125°C-275°C. For quartz reactions, stationary and rocked titanium alloy vessels filled with coarse Ottawa quartz sand are being used. Samples of reacted fluid are removed from the top of pressure vessels while fresh fluids are injected at the base. Quartz solubilities are being determined reversibly and the kinetics of the reactions are being outlined.

Ionization Equilibria in High Temperature Aqueous Electrolyte Solutions by Electrical Conductance Measurements (W. L. Marshall, J. D. Frantz, Geophysical Laboratory of Washington, DC)

Salts and other electrolytes in aqueous solutions are known to associate strongly at extremes of temperature (to 800°C) and at moderate to high pressures. The quantitative representation of this association and the determination of any possible hydrolysis of these electrolytes in high temperature aqueous solutions and supercritical fluids is of great importance for a full description in terms of the actual species present. The attainment of accurate ionization constants at extremes of temperature and pressure for particular acids and bases together with already available values for the ion-product of water and ionization constants for many salts previously obtained at ORNL will allow the above descriptions.

C. Geochemical Modeling

Stable Isotope Exchange in Mineral-Fluid Systems (D. R. Cole)

The isotopic ratios of $^{18}O/^{16}O$ and D/H have been increasingly used to resolve reaction paths of mineral-fluid reactions occurring both in the laboratory and in nature. This study is being undertaken to develop a basis for oxygen and hydrogen isotopic reaction kinetics in mineral-fluid systems undergoing mineralogic change. In addition, a detailed examination is made into factors that control diffusional isotopic exchange. Application of surface-controlled and diffusion models to well-studied geologic systems should prove useful in quantifying either time or water/solid mass ratios regardless of the degree of isotopic equilibrium.

Boiling and Mixing: Mechanisms for Self-Sealing in Geothermal Systems (S. E. Drummond and D. R. Cole)

Self-sealed zones are characteristic of many liquid-dominated geothermal systems and tend to occur at or near the margins of the reservoir. The processes of mineral deposition and rock alteration that lead to self-sealing have been attributed to the change from isothermal convection to a conductive gradient producing rapid temperature decreases, increased thermal fluid-groundwater mixing, boiling, and/or increasingly oxidizing conditions. Numerical models are being constructed to predict mineral solubilities in boiling and mixing hydrothermal solutions. These models are used to test the effectiveness of boiling or mixing as self-sealing mechanisms for a variety of well-documented geothermal systems. Results of these computations provide a quantitative understanding of the specific nature of natural boiling and mixing hydrothermal systems, ultimately leading to the development of better exploration criteria.

Contractor: PACIFIC NORTHWEST LABORATORY
Battelle Memorial Institute
Richland, Washington 99352

Contract: EY-76-C-06-1830

Title: I. Remote Sensing: Geoscience Data Analysis and Integration

Persons in Charge: G. E. Wukelic and H. P. Foote

Scope of Work

Since 1976, PNL has been conducting basic research in areas of remote sensing and image processing most relevant to the geoscientific research and development responsibilities of the Department of Energy. The basic purpose is to develop and test new interactive computer techniques for processing and using combinations of remote sensing and geosciences data so that geoscientists can analyze more complex data combinations, more completely and more rapidly.

The current scope and emphasis of activities involve:

1. Maintaining cognizance and acquiring appropriate remote sensing and geoscience data sets to support energy-related application efforts. Current emphasis is on acquiring Landsat-4 thematic mapper data and shuttle imaging radar data.

2. Upgrading computer capabilities (hardware and software) as required to advance the state of the art in digital processing, analysis and display of remote sensing (imagery) and geoscience (point, line and map) data. Near-term emphasis is on software development required to transfer existing interactive programs to the VAX 11/780.

3. Demonstrating, evaluating and transferring advanced computer techniques for processing and combining remote sensing and geoscience data of energy-related relevance. Current efforts involve cooperative assessments of potential utility to national security technology (with DOE/ISA), to Continental Scientific Drilling Program (with Sandia, Los Alamos and Livermore Laboratories), and to rock microstructure analysis (with Universities of Washington and Wisconsin).

A. Remote Sensing and Geoscience Data Base Expansion (H. P. Foote, S. C. Blair and G. E. Wukelic)

Each year, new data -- national, regional and local (Hanford) — are acquired and digitized as appropriate to support the development and demonstration of interactive computer procedures for merging remote sensing and geoscience data sets. As a Landsat-4 Principal Investigator, PNL is currently emphasizing the early acquisition and evaluation of the 7-band thematic mapper data over several geographic regions wherein DOE has geoscientific interests. These include several major operating facilities, such as Hanford and Savannah River Plants, sample nuclear waste repository locations and selected candidate Continental Scientific Drilling Program (CSDP) sites. PNL will be acquiring and processing Shuttle imaging radar data for geologic applications as they become available for selected areas of DOE interest. Also, acquisition of relevant geologic and geophysical data sets to support the preparation of CSDP demonstration products remains a high priority.

B. Software Development and Testing (H. P. Foote, S. C. Blair and G. M. Petrie)

Numerous specialized computer programs exist at PNL for interactively processing, enhancing and displaying remote sensing and geoscientific data. Current emphasis is on using these experimental programs to support other priority R&D interests of the DOE including the CSDP, expanded multispectral data use by ISA and potential contributions to geologic nuclear waste isolation activities.

Current work is underway to develop new programs to more effectively process and utilize the Landsat thematic mapper data being acquired for DOE by NASA, especially the new thermal band data. Research is also in progress to develop appropriate image processing techniques for analysis of microscale and macroscale geologic features. This work included a study of sandstones from the Illinois deep drill hole in which petrofabric data derived from image analysis will be compared with data derived using conventional methods in order to evaluate performance of the image processing technique. In addition, potential techniques for automatic grain classification such as multiband analysis will be evaluated.

C. Application and Transfer and Geodata Capabilities (H. P. Foote and G. E. Wukelic)

Previous demonstrations, reciprocal visits and data exchanges between PNL and other DOE National Laboratories involved in OBES geosciences programs have shown that PNL-developed geoscience computer processing (geodata) techniques could be beneficially applied to a variety of ongoing research and programmatic activities. More serious considerations and discussions are in progress to explore and develop procedures for accomplishing the transfer of appropriate capabilities.

Contractor: PACIFIC NORTHWEST LABORATORY
Battelle Memorial Institute
Richland, Washington 99352

Contract: EY-76-C-06-1830

Title: II. DOE Insolation/Aeronomy Observatory Studies

Person in Charge: G. M. Stokes and E. W. Kleckner

Scope of Work

The current program concentrates on the areas of aeronomy in the upper atmosphere and on insolation and radiative properties of the lower atmosphere. In particular, the aeronomy program is concerned with energy transport and interactions within the complex interface between the plasmasphere/magnetosphere regions and the ionosphere/upper atmospheric regions. Significant advances have been achieved over the past two decades in expanding our basic knowledge of the earth's atmosphere and magnetosphere and the sun as an interacting system. It is important that the physics of this coupling region be well understood in order to obtain definitive solar-terrestrial cause-effect relationships.

The insolation program relies on a data base of direct and diffuse solar radiation measurements made in visible and near-infrared spectral passbands. The research focuses on two goals. One is to quantify the spectral characteristics of scattered and direct sunlight. This is germane to energy generation solar technologies including photovoltaics and biomass and to passive solar technologies such as daylighting. The primary emphasis of the insolation task is on the characterization of the influence of trace species in the troposphere and lower stratosphere on solar radiation. These man-made or naturally produced trace species include aerosols, molecules and clouds.

A. Insolation Studies (J. J. Michalsky, N. R. Larson, G. J. Schuster, G. M. Stokes, and E. W. Kleckner)

The emphasis of the aerosol portion of the trace species work was intended to be an assessment of the human influence, including fossil energy technologies, on the environment. However, through volcanic activity, nature has masked any anthropogenic effects in the last three years. A study of the short-term tropospheric and longer-term stratospheric effects of the neighbor volcano Mount St. Helens has been completed and published in the Journal of Climate and Applied Meteorology. The major conclusion of this work was that the 1980 eruptions had no long-term climatic impact. Of greater consequence are the 1982 eruptions of El Chichon. Aerosol data have been collected at PNL radiometer sites in the northern hemisphere since the spring of 1978. Based on this data set which establishes background levels, it is easily determined that El Chichon continues to significantly perturb the stratosphere ten months after its eruption. From the attenuation of direct sunlight as a function of wavelength and from the breadth and displacement from the sun of the corona caused by diffraction by these stratospheric particles, a size distribution is to be determined. This result along with global distribution of the aerosols will ultimately determine the climatic impact of this volcano.

The extraction of information on trace gases depends on deviations from the expected smooth wavelength dependence of aerosol attenuation. Work continues on the validation of the PNL ozone extraction technique using the nearly colocated Boulder, Colorado, radiometer and the NOAA ozone network Dobson photometer. Several existing methods are being scrutinized to determine water vapor abundance.

Spectral data in seven broadband filters which span a silicon PIN diode's sensitivity are made every five minutes with a 1.5° field of view centered on the sun's disk. Less often scattered light measurements of the entire sky are made with approximately 10° between samples. Two mathematical approaches have been used to obtain continuous spectral distributions from these seven samples. Very good agreement with simulated, but realistic, spectra generated by the AFGL's LOWTRAN5 model has been obtained. Total irradiance values within one percent are obtained and reasonable averaging over spectral features yields spectra which should prove useful to materials, biological, and solar technologies. Validation using actual PNL radiometer measurements compared to LOWTRAN5 and absolute spectroradiometers at DSET Labs and SERI is in progress. A spectrometer for precision measurement of the transmission of optical elements has been interfaced to a computer. This transmission measurement is crucial in applying the mathematical inversion schemes.

B. Aeronomy Studies (E. W. Kleckner, D. W. Slater, and N. R. Larson)

The importance of mid- to high-latitude auroral and ionospheric phenomena has gained greater appreciation as evidence regarding the wide ranging and complex interactions has become available. The Stable Auroral Red arc (SAR arc) is among the variety of auroral emission patterns which occur frequently but are not visible to the naked eye. This phenomenon has been the subject of investigation for several years. As a result of this effort, PNL has produced the most comprehensive catalog of SAR arc events available to researchers. Dissemination of this unique archive has been achieved through publication in the open literature, and as continuing updates (through 1982) available as PNL reports.

SAR arcs are spatially associated with the equatorial plasmapause region of the magnetosphere and constitute the optical manifestation of energy flux to the ionosphere from that region. We have found that the energy dissipation within the ionosphere appears to be reasonably well explained; however, the energy transfer mechanism within the magnetosphere responsible for the maintenance of SAR arcs is yet to be adequately defined and, at the present time, is under active study. A cooperative study led to calculations of electron heating rates and temperatures within the body of a SAR arc. The results were then compared to our absolute photometric observations of integrated emission intensity. Good agreement was found between the calculated and observed emission rates.

A second study used the photometric network data in conjunction with Fabry-Perot interferometer measurements, the objective being a determination of the thermospheric response to energy input from both SAR arcs and the more poleward aurora. This has led to the first report of thermospheric winds resulting from SAR arc heating exclusive of competing aurorally generated circulation. In accordance with model predictions, measurements both North and South of the arc showed flow patterns

consistent with areas of subsidence of the thermospheric neutral oxygen, indicating that a thermal convection cell had indeed been generated. The modeled and observed behaviors in the vicinity of the arc were in close agreement.

In perhaps the most surprising and consequential study, in situ measurements by satellite above the locations of several SAR arcs have allowed identification of the low energy thermalized electron population believed responsible for the creation of the features. Analysis of the available data sets reveals a 1-to-1 correspondence in the occurrences of low energy electrons (<3 eV) and the locations of SAR arcs. The electron populations thus far examined exhibit field aligned convective velocities of 200-300 km/sec. Viewed from the plasma rest frame, calculations show that the convecting electron population above the arcs is well described by a Maxwellian thermal distribution with a characteristic temperature of ≈10,000 K.

A goal of the aeronomy program is to develop a capability to model the physics of the F-region in the ionosphere. This model, together with the extensive observational base, will provide a tool for detailed study of energy transport within this region. As a supplement to existing instrumentation, a compact and portable, 4-color meridian scanning photometer is under construction. This instrument will allow the acquisition of simultaneous absolute emission intensities at a number of auroral wavelengths. These ratios, in turn, will allow very specific particles within this region. A "core" network of three photometer sites located near PNL will continue to be operated so as to provide the high spatial resolution needed for studies of D- and E-region phenomena (≈100-km height).

Contractor: PACIFIC NORTHWEST LABORATORIES
Battelle Memorial Institute
Richland, Washington 99352

Contract: DE-AC06-76RL0 1830

Title: III. Chemical Migration by Contact Metamorphism in Granite - Carbonate Rocks

Person in charge: J. C. Laul

Scope of Work

The main objective is to investigate the relative migration and transport mechanism of major, minor, and particularly trace elements during contact metamorphism between granite and silt/carbonate rocks and granite pegmatite and country rocks. Specific emphasis will be on the rare earth elements (REE) -- Ba, Sr, K, As, Sb, Pb, Cl, Rb, Cs, Zr, Hf, Ni, Th, and U. The applications of this study may enable us to understand and predict the long-term (10^3 to 10^7 years) behavior and movement of radionuclides in geologically confined nuclear waste.

The first geological site has been the granite intrusion at Notch Peak, Delta, in western Utah. The intrusion was emplaced in a Cambrian limestone interbedded with silt and carbonate layers. Samples of silt and carbonate, ranging from highly metamorphosed (near contact) to unmetamorphosed, were collected along horizontal and vertical traverses away from the granite intrusion in the Big Horse, Weeks, and Marjum formations. Analyses on some 40 major, minor, and trace elements is obtained by neutron activation analysis and x-ray fluorescence. A comparison of trace element signatures from metamorphosed to unmetamorphosed samples, ranging from granite to silt/carbonate in the Big Horse formation, indicate that some elements -- Na, K, Rb, Ba, Sr, Cs, As, Sb and Pb -- in the silt have migrated over distances of 5-40 meters, whereas there is virtually no migration of REE, V, Cr, Sc, Zr, Hf, Al, and Th. Carbonate rocks are impermeable to fluids relative to silt. The chemical systematics of the Weeks and Marjum formations are under study.

The second geological site is pegmatite country rocks in the Black Hills, South Dakota. The five different pegmatites chosen will enable us to address (a) composition of fluids (b) capability of dispensing fluids into country rocks and (c) partitioning of mobile elements between minerals phases and fluids derived from pegmatites. Preliminary study on the Tin Mountain pegmatite suggests that K, Rb, Cs, and Sb have migrated to distances of $\sim$5 meters from the pegmatite/amphibolite contact. There is virtually no migration of REE, Al, V, Cr, Sc, Hf, and Th. The chemical study of mineral separates biotite and muscovite and concentration profile as a function of distance in other pegmatites is under progress.

This study is in collaboration with J. J. Papike of South Dakota School of Mines and Technology, Rapid City, South Dakota, who will obtain petrographic, petrologic, and isotopic systematics on the same samples.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Title: I. Magma Energy Research

Person in Charge: W. C. Luth

Scope of Work

The Magma Energy Research Project has been assessing the scientific feasibility of directly extracting energy from buried magma sources and has been divided into five major research tasks: magma source location and definition, magma source tapping, magma characterization, magma-material capability, and energy extraction. Magma Energy was judged to be scientifically feasible last year. Continuing research is following on the task of locating and defining specific shallow crustal magma bodies for future scientific/engineering experiments. Sites are being studied for future shallow magma experiments, and geophysical techniques for detecting shallow magma sites are being evaluated.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Title: II. Continental Scientific Drilling Program
Thermal Regimes

Person in Charge: W. Herrmann

Scope of Work

Research conducted under the auspices of the Continental Scientific Drilling Program (CSDP) - Thermal Regimes sub-program at Sandia involves both generic and site specific activities as well as technology development and operation of a Thermal Regimes Research Drilling Office. Generic supportive research efforts include: development and testing of advanced thermal geophysical techniques; analysis of surface manifestation of subsurface magmatic emplacement; and a portion of the research conducted under IV (Geochemistry Research) bearing on energy and mass transfer within, and between, hydrothermal and magma systems. Site specific research is concentrated at the Mono Craters-Long Valley, California, site and involves a number of non-Sandia participants. Recognition of the need for advanced technology to obtain scientific data in the hostile hydrothermal-magma transition zone resulted in a research program in drilling, logging and instrumentation to provide the base for technology development. A Research Drilling Office has been established to implement the drilling activities of the CSDP-Thermal Regimes sub-program. The first major activity of the Research Drilling Office will be to provide support for the joint laboratory (SNL, LANL, LBL, LLNL) shallow drilling research program.

A. CSDP - Thermal Geophysical Techniques (J. C. Dunn and H. C. Hardee)

The objective of this research is to develop and refine thermal geophysical techniques in order to characterize and understand in situ thermal processes in permeable convecting geologic media. Such thermal geophysical techniques are based on the measurement and analysis of thermal and fluid transfer, but particularly in regions where natural convection heat transfer and/or ground water flow in aquifers significantly alter subsurface temperature profiles. Current research is concentrating on the design of a convective heat flow sensor for use in permeable convecting surface zones. Initial tests were run at Long Valley and additional tests of an improved tool are planned later this year at Long Valley.

B. Magmatic Emplacement (C. R. Carrigan)

A primary objective of the CSDP is the characterization of the geology and physics of a geothermal system. A study is in progress to utilize the surface evidence of geothermal systems such as heat flow, gravimetric and tilt data to provide assessments of the present state and evolutionary track of these systems. This study is evaluating the effect of the coupled magma/wall rock and magma/hydrothermal interaction on surface observables. Numerical codes are being used to investigate evolutionary models of both resupplied and isolated magmatic structures such as dikes, sills, conduits, and chambers.

C. CSDP - Mono Craters-Long Valley (CA) Site Assessment (J. C. Eichelberger and J. B. Rundle)

In view of its long and intense history of volcanism and current seismic, tectonic, and fumarolic activity, the Mono Craters-Long Valley area is an important potential site for deep exploration of crustal thermal regimes. To assess this potential and to gain a basic understanding of magma/ hydrothermal systems, a coordinated program of geophysical and geochemical observation and modeling is being conducted. Intersecting refraction profiles have been completed across western Long Valley caldera and the Mono vent chain to define upper crustal structure. High precision gravity measurements, repeated over a network of benchmark stations, have recorded changes associated with recent seismic events. These events, possibly reflecting shallow intrusion of magma, were also observed through rapid deployment of seismic arrays. Analysis of carefully sampled suites of recently ($\leq 10^3$y) erupted glasses indicates important chemical and isotopic changes during magmatic intrusion and eruption, apparently as a consequence of degassing. Modeling efforts are underway to relate these surface observations to behavior of magma and hydrothermal systems at depth.

D. CSDP - Drilling, Logging and Instrumentation (H. C. Hardee and J. C. Dunn)

Drilling, logging and instrumentation support is concerned with developing advanced logging tools and downhole instruments for CSDP and then applying these tools to answer scientific questions of interest to CSDP. Early work has concentrated on downhole seismic tools and downhole high temperature thermal probes. Shallow test holes were drilled at Long Valley for the purpose of evaluating these logging instruments.

High Temperature (1200°C) thermal probes and associated cables and handling equipment are being developed for logging high temperature holes. Initial instrumentation work has concentrated on the development and testing of downhole periodic seismic sources. Both compressional-wave and shear-wave (P and S) sources have been developed. A swept-frequency periodic source is currently under development.

E. CSDP - Shallow Hole Investigation of Long Valley, Valles and Salton Sea Thermal Regimes (J. C. Eichelberger)

The intrusion of magma into the upper crust, the release of heat and volatiles from these intrusions, and the development of associated hydrothermal systems are problems central to understanding the evolution of continental crust and its resources. Recent research into magma/hydrothermal systems under the Continental Scientific Drilling Program have concentrated on Long Valley caldera, Valles caldera, and the Salton Sea. All three areas contain major, recently active magmatic systems and currently active hydrothermal systems. A general reconnaissance phase of work is well advanced at these sites and has defined specific questions which can be addressed by shallow drilling. These questions involve the mechanical, chemical (particularly with respect to volatiles), and thermal behavior of magma at shallow depth, and the composition and circulation pattern of hydrothermal fluids. An interdisciplinary and interlaboratory program of investigations in shallow holes is underway at these three candidate Continental Drilling sites as a necessary step toward deep drilling at these sites. Drilling targets are the conduits beneath the youngest vents at Long Valley and Valles calderas, and an unexplored region of the Salton Sea thermal anomaly. Laboratories participating in this proposal are Lawrence Berkeley, Lawrence Livermore, Los Alamos and Sandia National Laboratories. Sandia will have responsibility for drilling the vent at Long Valley and for interpreting petrologic data from the Long Valley and Valles holes in terms of the degassing of rhyolitic intrusions. Measurement of material properties of core and downhole geophysical experiments will be conducted in collaboration with the other laboratories in order to determine mechanism and rate of heat transfer and define conduit geometry.

F. Thermal Regimes Research Drilling Office (R. K. Traeger)

This activity will provide logistical support for research drilling programs in the CSDP-Thermal Regimes area. The support functions include consultation with principal investigators (P.I.'s) and program officers regarding budgetary and technological constraints on research drilling and aiding in the formulation of detailed drilling, logging and experimentation plans. The drilling office, if requested, will assume responsibility for environmental, safety, legal, and insurance activities associated with drilling programs, issue and monitor contracts for site preparation and field activities associated with drilling, provide (if necessary) a site engineer, and generally support the scientific activities of the P.I. and co-workers. The drilling office will provide support for a Scientific and Technical Review Panel which is charged with overall review of the research drilling activities.

G. Long Valley-Mono Craters (CA) Information Base (J. C. Eichelberger and J. B. Rundle)

An integrated information base containing references to published geologic, geophysical and geochemical data and interpretations is essential in considering detailed site selection for CSDP-Thermal Regimes. The information base will contain:

(1) Bibliographic information in standard reference format with keyword-based identification of data presented in the reference.

(2) A listing of researchers who are currently engaged in active research in this area, with a brief statement of type, nature, extent, and objectives of the research.

(3) Brief summary of generalized plans for future research, including shallow, intermediate and deep drilling.

The Information Base will be prepared on a stand-alone microcomputer using a conventional commercial data base management system. Information will be distributed in printed form on a semi-annual basis.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Title: III. Geophysics Research

Person in Charge: W. C. Luth

Scope of Work

Research in geophysics under this program involves modeling, experimental, and field activities leading to a more soundly based understanding of physical and mechanical processes in the earth's crust and upper mantle.

A. Crustal Strain (J. B. Rundle)

The purpose of the crustal strain program is the development of methods and techniques for interpreting time-dependent deformation of the earth's surface. Motions of a few centimeters a year, commonly observed in tectonically active areas such as the western United States, have been interpreted as due to subtle stress relaxation processes deep within the earth. These notions provide clues to the occurrence of a future event.

Computer codes have been developed which compute time-dependent surface deformation due to various sources in a layered, inelastic earth model. Additionally, other codes compute gravity, sea level, potential, and surface deformation changes due to volcanic loading of the crust; and heat flow, fluid flow and deformation due to sources of fluid pumping in a fluid-infiltrated work model. Gravity gradient data associated with the 1975-1977 Kilauea inflation-deflation episodes have been interpreted by use of these techniques. Work using these codes is underway with collaborators at the U. S. Geological Survey and at the Earthquake Research Institute, Tokyo, Japan. Seismicity data, waveform modeling and laboratory studies of rock deformation and slip suggest that shear stress is distributed inhomogeneously on fault planes. A model consisting of a finite fault embedded in an elastic medium has been constructed to explain these data.

B. Time-Dependent Deformation and Fracture of Brittle Rock (L. S. Costin and D. J. Holcomb)

This research is directed toward a basic understanding of the mechanics of microcrack growth and how this is reflected in the continuum response of the material. Both experimental and analytical efforts are in progress. An experimental determination of the relationship between applied stresses and the time-dependent growth of cracks in granite and marble has been established and shown to be consistent with the notion that time-dependent crack growth occurs by the mechanism of stress corrosion. In these experiments, both temperature and moisture were varied.

To apply the experimental results to the problem of time-dependent deformation of brittle rock, a relationship between microcrack behavior and continuum behavior was established through an analytical model based on fracture mechanics theory. Stress-strain curves for various loading histories are being predicted and compared with experimental results.

Currently efforts are concentrated on applying the model to long-term creep problems and experimentally verifying the results, extension of the model to a fully three-dimensional description and definition of damage accumulation inferred from acoustic emissions.

C. Creep Resonse of NaCl at Low Stresses and Temperatures (D. H. Zeuch and W. R. Wawersik)

The objective of this program is to investigate the creep mechanisms of sodium chloride at low temperatures and stresses. The creep response of sodium chloride has been studied extensively at temperatures above approximately one-half the absolute melting point, where it appears that dislocation climb is the creep mechanism; however, relatively little work has been carried out at lower temperatures. Such results as are available suggest that the dominant creep mechanism under lower-temperature conditions may be a thermally activated glide or cross-slip process. This in turn implies that creep history and initial substructure may exert a profound influence on the creep behavior of sodium chloride, because recovery is (implicitly) slow.

Work is in progress to conduct creep experiments on sodium chloride single crystals under low stress, low temperature conditions outside the range of any previous testing. Single-stage creep tests will be performed to assess the basic creep properties and substructural evolution of the single crystals. In addition, multistage temperature and stress-changing experiments will be carried out to determine the activation parameters and stress dependence of creep in order to: (1) identify the deformation mechanism(s); (2) quantify the kinetics of recovery; and (3) determine the influence of initial substructure on creep.

D. Natural Convection in Double-Diffusive Counter-Buoyant Systems (D. B. Hayes and J. C. Eichelberger)

In double-diffusive counter-buoyant fluid systems, gradients in temperature and composition produce opposing buoyancy forces, resulting in complex patterns of circulation. For example, heat is lost from the margin of a magma body but water may diffuse inward, resulting in opposing buoyancy forces within chemical, and thermal boundary layers of greatly differing thicknesses. The equations describing non-equilibrium flow of fluid (gas) - magma mixtures in conduits have been developed for the case involving low volume fraction of gas. Numerical solutions for these integro-differential equations, expected to be stiff because of disparate length scales, are being sought.

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Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Title: IV. Geochemistry Research

Person in Charge: W. C. Luth

Scope of Work

Research under this program involves experimental, analytical and theoretical geochemistry relating to magmatic and hydrothermal processes taking place within the earth's crust.

A. Hydrothermal-Magma Systems (W. C. Luth, T. M. Gerlach, J. C. Eichelberger, and H. R. Westrich)

This research is directed toward developing an understanding of mass and energy transport within and between hydrothermal and magma systems through a combination of field, experimental and modeling approaches. The research includes electron microprobe analysis of quenched in situ samples of basaltic magma obtained from drilling programs at Kilauea Iki Lava Lake in 1978 and 1981 as part of the Magma Energy Research Program, experimental studies of bubble nucleation and growth in silicic melts, studies of the amounts and kinds of volatiles in young silicic volcanic suites, and the chemistry of volcanic gases including sublimate and condensate fractions. Advanced methods are being developed for use of the fully automated electron probe in geochemical analysis of drill core samples. Computer software is also under development for processing and evaluating large data bases of automated probe analyses with complete propagation of error capabilities. Water contents are being determined for a large number of obsidian samples from explosively and effusively erupted young volcanic units at Mono Craters/Inyo Domes, Katmai, and the Cascade Range. These studies have focused on the isotopic composition and amount of water in the obsidian samples as a function of time. The rates of bubble nucleation and growth as a function of water content are being investigated in small plates cut from the same obsidian samples. Field, analytic, and computer-based studies of volcanic gases are being performed for Mount St. Helens and Kilauea Volcano in an effort to better understand chemical trends during magma degassing.

B. Clay-H_2O Interactions (J. L. Krumhansl)

The ability to predict the course of rock-water interactions at temperatures up to 350°C is critical to a number of geochemical, geophysical and energy related problems and to a large degree depends on a knowledge of the kinetic and thermodynamic constraints governing clay mineral dissolution. To approach the problem experimentally, a hydrothermal Dickson Apparatus has been brought on line and the requisite solution analytic equipment purchased and installed. Preliminary experiments using Wyoming bentonite demonstrated the desirability of eliminating exchangeable potassium and magnesium as well as amorphous silica in order to obtain readily interpretable changes in fluid composition. A theoretical methodology for dissolution data interpretation has also been located and a data base containing the appropriate thermodynamic values identified. Currently preparations are underway to program this theoretical model and for starting in earnest the hydrothermal experiments using the reference montmorillonite clay SWy-1.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Title: V. Advanced Concepts

Person in Charge: W. C. Luth

Scope of Work

Research conducted in this program involves exploratory research in several geoscience areas. Typically such research efforts are of a short-term nature and may be oriented toward assessing feasibility of a particular research task.

A. Field Portable Gas Chromatograph (R. O. Woods)

Efforts to characterize fumarolic gases by bottle sampling are perturbed by the reactive natures of the species involved. These cause deterioration of samples between the time of their being taken and their later analysis in the laboratory. In situ analysis using portable instrumentation avoids this problem. A field gas chromatograph, configured to analyze the gases commonly found in volcanoes and constructed of materials capable of surviving in a corrosive atmosphere, is being developed. To date the analytic instrumentation has been built and partially tested. The ongoing effort involves assembling a supporting electronics package and calibrating the overall system.

B. Mapping Damage Space in Rocks Using Acoustic Emission (D. J. Holcomb)

A technique is being investigated for studying the local failure processes that lead to macroscopic failure of polycrystalline materials, such as rock. Failure of brittle rock is the end point of a process of accumulating local failures which can be characterized with the concept of damage. If damage is a state variable, then it should be possible to map damage-stress space with acoustic emissions (AE) in a manner analogous to mapping yield surfaces for a plastic material. To show this, surfaces of constant damage are being mapped by approaching the surface along different stress paths, using the onset of acoustic emission activity as an indicator that the surface had been reached.

Preliminary results indicate that for the simple triaxial stress state, there are indeed "damage surfaces" that are detectable using acoustic emissions. An unexpected development was the realization that the same approach could be used to determine in situ stresses without the drawbacks inherent in other methods.

Continued development and generalization of the techniques is planned, applying the damage mapping methods to several rock types, using sufficiently general stress states that the full damage surfaces are delineated and integrating the results into existing failure models that are based on the concept of damage as a state variable.

C. Noble Metals (H. W. Stockman)

This study is directed toward defining the distribution of noble metals in the mantle. It is generally agreed that the distribution of noble metals among sulfide, oxide, and silicate phases in the mantle is an important factor in the production of noble metal-rich magmas, hence in the production of magmatic platinum-gold deposits. Work in progress involves both chemical analyses of natural materials and experimental studies of phase equilibria. A homogeneous, contamination-free and alteration-free peridotite standard has been prepared to test noble metal analysis techniques. Methods have been developed for separation of sulfides from mantle-derived rocks, and the sulfides will be analyzed to assess their contribution to whole-rock noble metal content. Experimental work includes determination of noble metal solubility in Fe-Ni sulfides, and redetermination of the Ru-RuS_2 sulfur buffer.

PART II

OFF-SITE

Contractor: UNIVERSITY OF ALASKA
Geophysical Institute
Fairbanks, Alaska 99701

Contract: DE-AT06-76ER70005

Title: I. Magnetosphere Annihilation and Applications

Person in Charge: S. I. Akasofu

Scope of Work

Plasmas in thermonuclear fusion research devices and in space around the earth have much in common. The earth's magnetosphere provides a unique opportunity to study some of the basic characteristics of plasmas, without complexities associated effects of the wall of fusion devices. One can also learn basic processes associated with the natural dynamo (consisting of the solar wind and the magnetosphere) which can generate as much as one million MW. Specifically, University of Alaska researchers are working with thermonuclear fusion groups at the University of Texas, Austin, and the Plasma Physics Laboratory, Princeton University, in applying computational methods developed by them to learn some of the basic characteristics of plasmas in nature.

University of Alaska researchers are also interested in energy-related geophysical problems in the Arctic region. In particular, they are studying the electric current induced by auroral activity in power transmission lines and in oil/gas pipelines. We have successfully demonstrated that auroral activity causes surges in the protective relay system in power transmission lines. An intense surge will open the protective relay, causing a system blackout; blackouts caused by auroral activity are fairly common in Canada where many power transmission lines are rather long. By studying the characteristics of the surges, we are designing a protective relay system which will not be affected by auroral activity. This project is important for the proposed Anchorage-Fairbanks tie line. Intense electric currents (as much as 1000 A at times) in an oil pipeline, induced by the aurora, may cause serious corrosion of the pipe. Geomagnetic disturbances at Prudhoe Bay also cause serious problems in the operation of various drilling sensors which are oriented by a magnetic compass. We plan to develop a feedback system to make necessary corrections automatically.

In the arctic region, permafrost provides serious obstacles in energy search and oil transport efforts. Thus, the determination of thickness of permafrost is increasingly an important problem. We have an impulse radar (GSSI), loop-loop induction systems (EM-31, -34), audio magnetotelluric systems, and electrical resistivity devices. We plan to cross-calibrate these instruments at locations where permafrost thickness and distribution are known by developing numerical methods to handle the data from all the radar and EM devices.

Contractor: UNIVERSITY OF ARIZONA
Department of Geosciences
Tucson, Arizona 85721

Contract: DE-AC02-81ER10842

Title: I. Rock Deformation in Magma Hydrothermal Systems

Person in Charge: Denis Norton

Scope of Work

The object of this project is to reconstruct the state of stress in magma-hydrothermal systems using field data and transport theory. We are using photogrammetric mapping methods for the collection of data on fractures in fossil magma-hydrothermal systems. Fracture characteristics such as frequency, spacing, continuity, and effective aperture are being mapped in one fossil system in detail and in several systems at a reconnaissance scale. New computer techniques are then being used to summarize data in the form of graphic images that will benefit engineers concerned with waste repositories and geothermal systems and that will improve the theoretical basis for analyzing processes in magma-hydrothermal systems.

We have developed a mapping method for accumulating information on the geometry of fracture surfaces found in fossilized magma-hydrothermal systems. The mapping system prepares three-dimensional models of outcrops and information contained within outcrops. These geometric images are then used to reconstruct the geologic history of a system by comparative analysis with mathematical models of the processes believed to have formed the system.

The data required for these studies are collected in steps: First, a preliminary geometric model of the important geomorphic land forms and structural elements is generated, using at least two high-quality photographic perspective images and a precisely surveyed control network of object coordinates. Second, this model becomes a base map on which the relative age, mineralogy, detailed fracture characteristics, and location of hand samples are annotated. Last, the preliminary model is refined using the new information above and extrapolating the fracture surfaces into the interior of the outcrop.

We are now applying this mapping system to studies of fossil magma-hydrothermal systems. This work has progressed to the stage of final computation and production of computer images in the field data. Preliminary images of topographic surfaces have been digitized; these will be used as the base surfaces on which outcrop information will be depicted.

The imagery ultimately collected from field sites contains numerous features of interest that will be transformed into computer images. Although the computer processing is as yet incomplete, there are many qualitative aspects of the images relevant to the academic and engineering goals of our research.

Contractor: UNIVERSITY OF ARIZONA
Tucson, Arizona 85721

Contract: DE-AC02-80ER10753

Title: II. Solar Variability: Figure and Mean Diameter

Persons in Charge: H. A. Hill and R. J. Bos

Scope of Work

The objective of this work is to develop and utilize an indirect diagnostic of solar constant changes through changes in the solar shape and mean diameter. The search for indirect diagnostics of luminosity is motivated by difficulties in obtaining reproducible radiometer data over the years to decades associated with terrestrial climatic changes. During the 1970's, SCLERA developed techniques to measure fractional solar diameter changes to accuracies of $\Delta D/D \approx 10^{-5}$ to 10^{-6} over a one-day observing run ($\sim$ 9 hr). These techniques will be extended over climatically significant timescales. The relationship between the indirect diagnostic and the solar constant is also being examined theoretically.

A. Technical Developments

A system is now being constructed to calibrate the telescope field absolutely to potential accuracies of 10^{-3} arcsec. The calibration is performed by interferometrically measuring angles between images in the telescope field produced by a single mode laser and a reflecting grating. The interferometer is also being used to monitor the shape of the limb scan, a modification which will reduce systematic errors below the level obtainable with the CID camera formerly scheduled for this purpose. Sophisticated lightning protection devices have been installed at the telescope site in order to minimize the possibility of future lightning damage.

B. Observations

A preliminary analysis has been completed of data taken in 1981, prior to the extensive damage caused by lightning. Analysis of these observations is continuing. The current observational run began in mid-May 1983. The new program utilizes four diameter measurements, a procedure which facilitates corrections for effects due to the earth's atmosphere. To minimize bias caused by rotation of the detector between the four different diameters, the data are to be Fourier analyzed as one linked set. The signal-to-noise ratio obtained using this technique has been found to be satisfactory.

C. Theoretical Work

A theory has been developed to treat properties of long and short period oscillations. The theory includes effects due to the mean intensity's nonlocal nature, deviations from radiative equilibrium, and a nongray atmosphere. For the long period oscillations of interest in studies of variability in the solar constant, the nonlocality of the mean intensity is the most important effect, producing percentage temperature changes 10^3-10^4 times larger than those occurring in the diameter. This theory has been used to intercompare results of diameter, Doppler, and radiometric studies of the 160 min period oscillation; agreement is found to be approximately within the limits of observational error. The 1979 observations also produced the discovery of rapid internal solar rotation, a finding with important implications for Einstein's general theory of relativity and other theories of gravitation.

Contractor: ARIZONA STATE UNIVERSITY
Department of Chemistry
Tempe, Arizona 85287

Contract: DE-AC02-80ER10765.A000

Title: Silicate, Aluminosilicate and Borosilicate Melts:
Thermochemical Studies by High Temperature Calorimetry

Person in Charge: A. Navrotsky

Scope of Work

High temperature solution calorimetry is used to determine heats of mixing in aluminosilicate glasses and melts. We are focusing on the role of oxide basicity in determining mixing properties along the joins $MAlO_2$-SiO_2 (M = Li, Na, K, Rb, Cs, Mg, Ca, Ba, Sr, Pb) and in determining heats of vitrification and of fusion. These systematics lead to an understanding of effective heats of fusion of diverse components in an aluminosilicate framework. In addition, we have completed study of the system $KAlSi_3O_8$-$NaAlSi_3O_8$-Si_4O_8 and are continuing the modeling of phase equilibria in silicate systems, using experimental heats of mixing and of fusion and models for entropies of mixing. The emphasis is on ascertaining the usefulness of the two-lattice model for the entropy of mixing and in developing more appropriate complex structural entropy models.

A pressure vessel for the study of heat contents of hydrous melts in the system $KAlSi_3O_8$-$NaAlSi_3O_8$-Si_4O_8 up to 1000°C and 1 kbar has been constructed. It will permit direct study of the thermodynamic properties of glasses and melts containing up to 50 mol% H_2O by drop calorimetry under high pressure. Calibration and testing of the equipment is underway. In addition, solution calorimetry of hydrous glasses may be feasible.

The data and models are correlated to the structure and physical properties of silicate melts and have potential application in such diverse fields as geochemistry, magma energy generation, ceramic science, nuclear waste disposal, and reactor safety.

Contractor: BROWN UNIVERSITY
Department of Geological Sciences
Providence, RI 02912

Contract: DE-AC02-79ER10401

Title: Major Volcanic Centers: Magnetotelluric Studies

Person in Charge: John F. Hermance

Scope of Work

The focus of activity at this laboratory is on applying geophysical and electromagnetic techniques to detecting and characterizing geological features and physical processes within the earth that are related to energy sources. Presently attention is being directed toward acquiring an understanding of dynamical processes and thermal regimes associated with centers of major volcanic activity, particularly the Long Valley/Mono Basin volcanic complex. This work is related to questions of basic scientific importance, as well as to national priorities in resource related areas such as geothermal energy, chemical transport of minerals in the crust, the emplacement of economic ore deposits, and deep drilling for scientific purposes. It is felt that to understand the dynamic evolution of intraplate volcanic centers in the western United States, it is necessary to understand the segregation of basaltic magma from parent mantle material at depth (30 to 100 km) and its migration to higher levels in the crust (5 to 15 km). The physical transport of molten material offers an effective mechanism for transferring heat from deep sources to shallow depths in the crust, leading in turn to episodes of crustal melting at shallow depth and silica volcanism at the surface. In addition, combined electromagnetic and seismic studies of the crust at depths less than 5 km can play an important role in characterizing the porosity and permeability of the crystalline basement above possible magma chambers. This information is important to understanding the manner in which active hydrothermal systems are dynamically coupled to magma sources at high levels in the crust; we need to identify whether the mechanisms for heat transport is through simple conduction or if it is through fluid-transport (advection or convection). In addition, geophysical constraints on the permeability of crystalline basement are important for characterizing the transport of chemical species in the crust (via ore-bearing fluids, for example).

A. Thermal Processes Associated with Major Volcanic Centers

Geophysical investigations of the major rift zones of the world typically indicate that all of these regions exhibit anomalously low values of electrical resistivity, density and seismic velocity, either within the crust itself or at high levels of the mantle. Beneath intraplate rifts such as the Basin and Range or the Rio Grande rift in the western U.S., the emplacement of basaltic magma at mid-levels in the crust may lead to extensive remelting, triggering eruptive episodes of silica magmatism, such as associated with the Valles caldera or the Long Valley/Mono Basin complex. However, the interpretation of magnetotelluric measurements made by our group in these two areas does not indicate a profound geophysical anomaly such as would be expected to be encountered if a major magma body were present. We feel, therefore, that silica magma centers, beneath resurgent calderas of this type, solidify very quickly after eruption. This requires a mechanism for renewing thermal activity at depth in the crust. We are pursuing this question through geophysical field work in the Long Valley/Mono Basin area, as well as in the Valles caldera. Preliminary inspection of data obtained during the 1981-82 field seasons suggests the presence of an anomalous conductor associated with the Eastern Sierra Front, but does not indicate the presence of a high level magma body associated with Mono Craters.

B. Physio-chemical Processes Associated with the Genesis of Primitive Crust

We are continuing our interpretation of geophysical/electromagnetic experiments on Iceland and adjacent areas of the Mid-Atlantic Ridge. A magnetotelluric field experiment was mobilized in collaboration with the Icelandic National Energy Authority during the summer of 1982. It verifies that crustal thickening due to underplating provides a significant contribution to mechanisms of crustal genesis in this region. According to this model, mantle derived melt accumulates in a thin layer at the base of the crust beneath the neovolcanic zone. With time, this melt cools, solidifies, and accretes to the base of the crust leading to crustal thickening. The crust increases in thickness from 8-10 km directly beneath the neovolcanic zone to an average value of 10 km for the generally older ($\sim$ 10 m.y.) Iceland plateau. Hence, segregation of material from a significant volume of the mantle and continued crustal underplating may persist well beyond the boundaries of surface manifestations of volcanic activity. There is a strong possibility that such a process may be operational beneath the Basin and Range Province and the Salton Trough in the western U.S.

C. Magnetotelluric/Magnetic Variation Field System

To investigate these phenomena, a geophysical field system (using tellurics, magnetotellurics and geomagnetic variations over the frequency range 10^{3} Hz to 10^{4} sec) has been developed under joint support of the Department of Energy Office of Basic Energy Sciences and several other Government agencies. A comparative study is being undertaken of selected major volcanic centers in the western U.S. in terms of their association with regional tectonomagmatic phenomena in the deep crust and upper mantle. This year Brown University completed the testing and development of a magnetotelluric field system which consists of a microcomputer-based (DEC, PDP 11/23) multi-component data acquisition system capable of real-time acquisition, analysis and display of magnetotelluric data in the field environments. The system, mounted in a 4-wheel drive GMC van, has been used for preliminary field work in the Mono Basin/Long Valley volcanic complex.

D. Theoretical Models of Electromagnetic Induction Phenomena

General

The application of geophysical techniques to problems in the field are often constrained by the adequacy of modeling algorithms necessary to interpret the actual data. Because of this we have devoted a significant part of our research effort to developing models to simulate the electromagnetic response of representative geologic structures.

Modeling Three-Dimensional Induction Effects

A new finite difference form has been developed for simulating the distortion of telluric fields by three-dimensional azimuthally symmetric structures. The technique involves a sequence of local integrations of the electric current density crossing closed surfaces surrounding each mesh mode. The resulting expressions, which are accurate to second degree everywhere, not only correctly describe first-order discontinuities in the electric field normal to electrical discontinuities in the interior of the model, but also lead to significantly improved accuracy near sharp, localized discontinuities where the anomalous field decays as $1/R^{2}$ or $1/R^{3}$ with distance. When numerical simulations are compared with analytical solutions for simple models, the analytical and numerical results for a thin disk indicates an rms-accuracy of 1%, whereas for an imbedded sphere the rms-accuracy is 2%.

Bias of Long-Period Magnetotelluric Response Parameters Due to Lateral Heterogeneities

A simple three-dimensional model has been used to evaluate the bias of long-period magnetotelluric principal resistivity values in the presence of modest current channeling at shallow depth. It was shown that conventional MT parameters are not always good indicators of the degree to which the observed resistivities depart from a quasi one-dimensional response function. Large skew is sometimes associated with minimal bias. But unfortunately, small skew is sometimes associated with maximal bias. Also it appears that the geometric mean of the maximum and minimum principal resistivity values at a site may be regionally biased in a statistical sense for a large number of sites. A smaller bias can be achieved if one can identify the class of conductivity structures associated with local perturbations of the long period response parameters.

Finite Source Fields Coupled to Lateral Conductivity Heterogeneities: Effects on Magnetotelluric and Magnetic Gradiometric Deep-Sounding Experiments

Studies of the dynamical evolution of source fields in the ionosphere and magnetosphere are in many cases incompatible with global scale sources. In some cases, source fields have coherent scale distances of only a few hundred km, even at low and mid-latitudes. The possible effects of these finite source dimensions on induction experiments therefore require renewed scrutiny, particularly as deep-sounding measurements are performed at periods greater than 10^4 sec. The magnetic variation gradiometric technique appears to suffer from source effects at least as much, and perhaps greater than, the magnetotelluric technique. When finite source fields are coupled to lateral heterogeneities, the interaction becomes quite complex. We are attempting to generalize concepts regarding the interaction between the spatial wave-length of the source field and the scale size of lateral heterogeneities.

Contractor: CALIFORNIA INSTITUTE OF TECHNOLOGY
Seismological Laboratory, Division
of Geological and Planetary Sciences
Pasadena, CA 91125

Contract: DE-AT03-83ER13120

Title: In Situ Stress in Deep Boreholes

Person in Charge: T. J. Ahrens

Scope of Work

Knowledge of the in situ stress field is important to our understanding of contemporary tectonic, geothermal, and rock-forming processes, and provides information which is required to exploit energy resources and store waste in the earth.

We are developing a new type of stressmeter which employs interference holography and by means of laboratory and field measurements attempting to turn it into a useful geophysical tool. However, we have not yet used it as it is finally intended to be used; that being to determine the six independent values of the stress tensor at one point and to routinely log many data points along a narrow (e.g., 6" diameter) borehole. We are currently carrying out tests with the present instrument in the laboratory and in a Colorado oil shale mine. We expect in the next year to design, construct and test a smaller 6" version of the present experimental apparatus and test it in the laboratory as well as a series of scientific drill holes near the San Andreas fault in Southern California.

Contractor: UNIVERSITY OF CALIFORNIA
Department of Physics
Berkeley, California 94720

Contract: DE-AMO3-76SF00034

Title: Isotopic Studies on Rare Gases in Terrestrial Samples and in Natural Nucleosynthesis

Person in Charge: J. H. Reynolds

Scope of Work

This project is concerned with research in rare gas mass spectrometry. The broad objective is to read the natural record that isotopes of the rare gases comprise as trace constituents of natural gases, rocks, and meteorites. In past years, these interests have led to the study of such diverse problems as the dating of rocks, the early chronology of the solar system as revealed by extinct radioactivities, and the elemental and isotopic composition of trapped primordial rare gases in meteorites. In recent years the project has focused progressively more on terrestrial problems.

Our current work for DOE is focused on the RARGA system, which is a self-contained, mobile laboratory designed to make precise elemental and isotopic abundance measurements of the noble gases in terrestrial fluids. Recently road tested, the lab will be deployed from July 1 to late October 1983 in Yellowstone National Park for a detailed study of the noble gases from hot springs in that important tectonic hot spot. Our preliminary work on Yellowstone samples has identified a radiogenic argon component that is closely correlated with mantle derived helium of high $^3He/^4He$ ratio. The use of such correlation techniques to identify gas components from the mantle or other well-characterized sources is an important thrust of our research. After the intensive study planned for mid-1983 at Yellowstone, we hope to have improved greatly our understanding of the various geothermal basins at Yellowstone, i.e., how they are related to one another and how they are coupled to mantle sources.

Another project (now in press) with RARGA concerns noble gas solubilities in brines. Those studies have provided thermodynamic data that can place constraints on the physical structure of gas-bearing solutions and help to model the transport of noble gases in natural hydrothermal circulation systems.

A RARGA manuscript in preparation concerns noble gases in water and steam samples from the Lardarello geothermal field in Tuscany, Italy. Helium isotopic, argon isotopic, and elemental data from all the noble gases vary considerably from sample to sample, with trends beginning to develop when the data are plotted versus position in the field.

Turning to other projects, we are studying the solubility of noble gases in silicate melts as a function of their temperature and composition. An isotopic dilution technique affords considerable precision in these measurements, which are being made in collaboration with the Carmichael group at LBL.

A study of noble gases in diamonds of two types and from a number of geographical locations is well underway, with numerous samples now on hand and a new furnace, for outgassing the diamonds without generating excessive blanks, under construction.

A collaboration with Craig's lab at UCSD has made definitive measurements, which are being readied for publication, on the isotopic composition of neon from submarine basalts.

A number of other projects are in preliminary stages, including work on samples from the Baca geothermal field in the Valles caldera, New Mexico.

Contractor: UNIVERSITY OF CALIFORNIA
Department of Geology and Geophysics
Berkeley, California 94720

Contract: DE-AM03-83ER13100

Title: Advective-Diffusion/Dispersion Transport of Chemically Reacting Species

Person in Charge: H. C. Helgeson

Scope of Work

This project is aimed at development of a comprehensive transport model for hydrothermal systems. The model will be used to describe mass transfer using an advection-diffusion/dispersion equation coupled to mass action equations representing reversible chemical reactions including aqueous complexing, oxidation/reduction equilibria, ion-exchange with stationary minerals, and precipitation/dissolution reactions. The numerical approach is based on an implicit finite difference scheme which provides for simultaneous coupling of fluid flow, diffusion, and chemical reactions. This method is superior in numerical stability and accuracy to its explicit analogs. The model will be used to interpret phase relations in hydrothermal/geothermal systems, weathering profiles, and altered sediments where quantitative comparisons can be made between the predicted and observed spatial distribution of secondary mineralization. More accurate calculations can then be carried out to evaluate the geochemical and environmental consequences of acid rain, reservoir flooding, and toxic waste disposal.

Contractor: UNIVERSITY OF CALIFORNIA LOS ANGELES
Institute of Geophysics and Planetary Physics
Los Angeles, California 90024

Contract: DE-AT03-81ER10965

Title: Adiabats and Grüneisen Parameter at High Temperatures and Pressures

Person in Charge: R. Boehler

Scope of Work

It is generally accepted that the removal of heat produced by radioactive sources from the earth's interior is only possible by a convecting mantle. Since the earth's mantle is convecting at a high Rayleigh number, a representative temperature profile for the mantle as a function of depth is probably following the adiabatic temperature profile closely over most of its extent.

We have calculated a thermal model for a three-layer mantle of a self-gravitating earth. The model is based on measurements of the adiabatic gradient at high pressure and high temperature of olivine and MgO and the empirical law $(\partial T/\partial P)_S = (\partial T/\partial P)_{S,O} \exp(m(V/V_O - 1))$ found from recent measurements on compressible materials, such as the alkali metals lithium, sodium, potassium, and cesium. The volumes were calculated from a first order Birch equation using laboratory data of B, the bulk modulus, and its pressure and temperature derivatives. $(\partial T/\partial P)_{S,O}$ was calculated from laboratory data on the density, specific heat, and the thermal expansion coefficient. The model yields the pressure, the acceleration due to gravity, the density, the adiabatic temperature, the Grüneisen parameter, the thermal expansion coefficient, and the isentropic bulk modulus as a function of depth. The temperature at 100 km depth is taken as 1600 ± 100K. From our calculations the adiabatic temperature gradient at the top of the upper mantle is 0.45 Kkm^{-1} and decreases to 0.21 Kkm^{-1} at the bottom of the lower mantle. The adiabatic temperature difference across the whole mantle is 780 ± 100 K. The Grüneisen parameter decreases from 1.17 to 0.92 in the upper mantle and from 1.44 to 1.00 in the lower mantle.

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Contractor: THE UNIVERSITY OF CHICAGO
Chicago, Illinois 60637

Contract: DE-AC02-80ER10763

Title: Water and Magma Bodies

Person in Charge: A. T. Anderson, Jr.

Scope of Work

The emplacement, crystallization and eruption of silicic magmas are important both for the compositional evolution of the crust as a whole as well as for the formation of a variety of ore deposits and geothermal fields. We are attempting to develop a new way to determine the pressures of crystallization within such bodies of magma. The new method relies both on the increased solubility of H_2O and CO_2 in silicate melts with pressure and on the preservation of samples of the natural high pressure environment of crystallization as tiny inclusions within virtually rigid crystals. We make wafers of the crystals found in silicic volcanic rocks to expose inclusions of glass for analysis both by the electron microprobe for major elements and by a special vacuum fusion device for H_2O and CO_2. So far we have made a few analyses of the glasses for both H_2O and CO_2 which suggest pressures of entrapment above 2 kbar (2×10^8 Pa). We are struggling to make these analyses more accurate (to about 0.1% H_2O and 0.01% CO_2). The principal problems are the difficulty of getting the gases completely out of the viscous melt in a way that yields a small enough blank. Results on two samples of the Bishop Tuff from California, suggest variable concentrations of H_2O and CO_2 in melt inclusions in quartz phenocrysts from different samples of the Plinian ash fall. We are checking our extraction techniques further in the light of this apparent, and unexpected variability. We hope to be able to confirm or improve Hildreth's estimates of the range of vapor pressures within the body of magma before its extrusion. Future studies may reveal the change in magmatic vapor pressures with time as the body of magma developed prior to the cataclysmic eruption. Comparison of such data with similar data on recent rhyolites from Mono Craters and the Inyo Domes may help assess the current state of the (Mammoth Lakes) magma body.

Contractor: COLUMBIA UNIVERSITY
Lamont-Doherty Geological Observatory
Palisades, New York 10964

Contract: DE-AS02-76ER03134

Title: I. Tectonics of the Eastern Aleutian Arc

Person in Charge: K. Jacob, E. Hauksson, and L. Sykes

Scope of Work

The physical processes associated with the tectonics of a classic, subducting plate margin and its volcano-magmatic arc are studied mostly by seismological methods. A 12-station telemetered seismic network with one- and three-component, short-period high-gain, and broad-band medium-gain sensor combinations with digital event-detection and digital recording provides the data for this basic tectonic study. The data are analyzed for velocity and attenuation structures in the crust and upper mantle from travel time and waveform information, for spatial distributions of seismicity in the subduction zone and volcanic arc using hypocenter locations, for deformation and stress patterns using focal mechanism solutions, and for the distribution of magma and its migration in the volcanic arc using all of the above methods. The seismic network is centered on the Shumagin Islands Seismic Gap, a >300 km-long arc sediment that has a 30 to 99% probability for a great (M_w ~8 or larger) earthquake to rupture the plate boundary during the next two decades.

Recent results have shown a northward dipping Moho structure in the forearc region; a systematic increase of stress drop with seismic moment of thrust zone earthquakes with magnitudes M_L = 2 to 6; a slightly enhanced seismicity at shallow depths (~25 km) and in the Benioff-zone (<250 km), that in time coincided with a geodetically detected, mostly aseismic slip event (amplitude 80 cm!) between the descending Pacific slab and the overriding mantle of the North American plate; the slip was restricted to depths between ~20 and ~120 km, and in time also coincided (1978-1980) with a two-year eruptive quiescence of the otherwise active Pavlof Volcano whose seismicity we monitor. The deep slip event further stressed the presently locked, shallow thrust zone and thus should have brought it closer to failure.

Although this study is focused on basic tectonic processes, important results concern the seismic, volcanic and tsunami hazards to offshore structures for oil exploration in outer continental shelf regions within and directly adjacent to the Shumagin seismic gap and network.

Contractor: COLUMBIA UNIVERSITY
Lamont-Doherty Geological Observatory
Palisades, New York 10964

Contract: DE-AC02-76ER04054

Title: II. Fluid Transport Properties of Rock Fracture

Person in Charge: T. Engelder and C. Scholz

Scope of Work

The problem is to completely characterize fluid flow within the crust of the earth both in space and time. Part of the solution is to simulate in situ conditions in the laboratory. Previous laboratory work on fluid flow within jointed rock has focused on the transport properties in space (the effect of pressure and temperature on mechanical properties of joints). Current laboratory work involves characterizing time-dependent changes of the transmissivity of joints (the effect of dissolution and precipitation on the joint openings).

The initial time-dependent transmissivity experiments have been run using Barre Granite and a pelagic limestone. The experimental conditions include confining pressure of 50 MPa, a pore pressure of 20 MPa, and a variety of temperatures to 150°C. The experiments have lasted up to eight days with flow rates driven by a pressure difference of about 0.5 MPa for the granite with a rough surface and 5 MPa for a limestone with a smooth surface. Flow rate for the granite increased with time whereas the flow rate within the limestone slowed with time. Surfaces were examined with a profilometer showing that the grain boundaries of the granite eroded with time thus increasing the aperture of the joint. Erosion of contact points on the limestone allowed the limestone to close in time. Chemical analyses showed that solubility of the granite increased with temperature.

As a continuation of our work on the time-dependent transmissivity of joints, we propose experimental and analytical investigations in five areas. The principal work is to document the effect of water rock interaction on joint transmissivity at various pressures and temperatures within the upper crust. Associated projects include analyzing the pore-fluid for major elements in solution as a result of the rock-water interaction as well as x-ray analyses of the minerals deposited on the joints. The surface topography of joints will be studied to understand the effect of topography of joint stiffness and the effective stress law of joints. In another study the effective stress law and the cubic law will be reexamined using nonreactive pore fluids. Finally we plan a study of the retention of radionuclides on rock fractures to assess the flow paths along joints of various roughnesses.

Contractor: HARVARD UNIVERSITY
Department of Geological Sciences
Cambridge, Massachusetts 02138

Contract: DE-AC02-83ER13096

Title: Energetics and Thermochemical Properties of Rocks and Minerals

Person in Charge: J. B. Thompson, Jr.

Scope of Work

Any thorough understanding of the earth's crustal processes and energy budget must take into account the energetics and thermochemical properties of rocks and their constituent minerals, notably heat capacities, and enthalpies and entropies of transformations. Some of the transformations of concern are homogeneous (structural changes within single mineral grains), others are heterogeneous, involving the appearance or disappearance of mineral phases of a given phase assemblage. Heating of many minerals results in the release of volatile species that may either create a fluid phase or add substance to a pre-existing one.

Much of the requisite thermochemical data to handle the above problems are unknown or inadequately known. We propose to augment the thermochemical data base for rocks and rock-forming minerals by high-temperature (25 to 1700°C) differential scanning calorimetry, coupled where appropriate with simultaneous controlled-atmosphere thermogravimetry. We also intend to investigate the energetics and kinetics of homogeneous transformations in important rock-forming minerals. In addition, the high-temperature heat capacities and heats of fusion of minerals and mineral series comprising certain igneous rocks will be investigated. The thermodynamic data and models generated from them not only are of concern to metamorphic and igneous petrologists, but have potential application in such fields as the extraction of geothermal energy, nuclear waste disposal, terrestrial heat-flow studies, and the geochemistry of ore deposits.

Contractor: UNIVERSITY OF HAWAII AT MANOA
Hawaii Institute of Geophysics
Honolulu, Hawaii 96822

Contract: DE-AT03-80ER12099

Title: Physical Characterization of Magma Samples

Person in Charge: M. H. Manghnani

Scope of Work

This project is concerned with two areas of laboratory investigation: (1) characterization of physical (density, porosity, and pore size distribution), seismic (V_p, V_s, Q^{-1}), and thermal (conductivity) properties of core samples from Kilauea Iki Lava Lake under in situ conditions, and (2) viscosity, electrical conductivity, and V_p, V_s, and Q^{-1} of magmatic fluids at elevated pressures and temperatures and as a function of controlled volatile (e.g., H_2O, CO_2) content.

The goals of the proposed research are threefold: (1) to understand how the physical properties of basalts relevant to geothermal exploration and thermal modeling in a volcanically active area are affected by a total environmental system; (2) to investigate interrelationships between the various properties; and (3) to correlate the laboratory data with the models based on theory and field measurements.

Two parts of the proposed work (chemical and mineralogical analyses of Kilauea Iki and other samples, and viscosity and electrical conductivity of magmatic fluids at elevated pressures) are being conducted in cooperation with the two groups headed by W. C. Luth and M. J. Davis at the Sandia National Laboratories. One of the motivations of the proposed cooperative research is the availability of the unique Magma Simulation Facility at the Sandia National Laboratories.

The physical, seismic, electrical and thermal properties (diffusivity, conductivity and specific heat) of selected Lava Lake core samples, for which chemical composition and mineralogy have been determined by the Sandia Laboratories (Dr. W. C. Luth), are now in progress. For a few of these core samples and the other basalts obtained from the Hawaii Geothermal Project-A (HGP-A hole), both thermal diffusivity and C_p have been determined as function of temperature to 750°K. Analysis of the thermal data will be made in terms of chemistry, glass content and mineralogy of these core samples.

Compressional wave velocity (V_p) and attenuation (Q^{-1}) measurements are proceeding on melts of two plagioclase compositions: $Ab_{80}An_{20}$ and $Ab_{50}An_{50}$, where Ab stands for albite ($NaAlSi_3O_8$) and An stands for anorthite ($CaAl_2Si_2O_8$). Plagioclase is among the major constituents of Hawaiian basalts. Ultrasonic measurements on $Ab_{80}An_{20}$ have been carried out at 1500°C over the frequency range 5-20 MHz. Measurements on $Ab_{50}An_{50}$ have been carried out at 1475 and 1500°C, over the same frequency range. The data indicate that for both samples the relaxation times are on the order of 10^{-7} second near 1500°C.

The proposed research, involving close cooperation between the University of Hawaii and the Sandia National Laboratories, is not only relevant to the ongoing research efforts of the Magma Energy Research program of the Department of Energy, but it also provides an impetus to basic energy research needed for acquiring a better knowledge of the fundamental in situ physical properties of rocks relevant to planned projects such as the U. S. Continental Scientific Drilling Program.

Contractor:	MASSACHUSETTS INSTITUTE OF TECHNOLOGY Department of Earth and Planetary Sciences Cambridge, Massachusetts 02139
Contract:	DE-AC02-76ER02534 A008
Title:	Seismology of Crack Formation
Person in Charge:	K. Aki

Scope of Work

This program was started as an involvement in two major geothermal projects, namely, the Hot Dry Rock Geothermal Energy Development Project of the Los Alamos National Laboratory and the Magma Tap Project of Sandia National Laboratories. The theory and methods developed for interpretation of various seismic experiments conducted at Fenton Hill, New Mexico, and Kilauea Iki, Hawaii, however, found a variety of applications to other geothermal areas and volcanoes, and our research has been evolving into what might be called Volcanic Seismology.

In this research program, we are interested in both passive and active seismology. We constructed a set of digital event recorders for collection of high-quality data as used in our study of Mt. St. Helens. Our interpretation methods for observed seismic signals from volcanoes and geothermal areas include the effects of seismic wave generation, transmission, scattering, and attenuation in a medium containing fluid filled cracks.

Our study areas include the hot dry rock fracture system at Fenton Hill, magma lens in Kilauea Iki, deep and shallow volcanic tremor sources under Kilauea, inside Mt. St. Helens, and Long Valley. We obtain data from our own event recorders as well as those collected by other universities and government agencies in the U.S. We are also collecting data from Mexico, Japan, New Zealand, and France through cooperation with universities and research institutions in these countries. We are also developing a borehole seismograph which can be operated at high temperature.

Contractor: MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Earth and Planetary Sciences
Cambridge, Massachusetts 02139

Contract: DE-AC02-78ER04972

Title: Microcrack Technology

Person in Charge: G. Simmons

Scope of Work

The objective of this project is to demonstrate the usefulness to the DOE energy programs of various aspects of microcracks in rocks. Open microcracks control such important properties as permeability, electrical conductivity, and velocity of elastic waves. Healed microcracks provide data on the history of the rock and evidence that may be useful for predicting future physical and chemical characteristics. Potential practical applications include site characterization for waste repositories, estimation of changes of permeability of rock in situ due to changes of temperature associated with production in a hot-dry-rocks geothermal system, prediction behavior of certain isotopes from radwaste in granitic rocks, and improvements in exploration techniques for uranium in crystalline rocks.

We use the petrographic microscope, the scanning electron microscope (SEM) equipped with both high energy resolution backscattered electron detector and imaging system and an energy dispersive x-ray system, and various physical properties measured as a function of pressure to characterize microcracks. The SEM yields information on healed cracks (composition and extent of the minerals that fill formerly open microcracks, extent of healing, and the physical dimensions). Presently open microfractures are characterized with the SEM and also with a high precision technique for the measurement of strain as a function of pressure (differential strain analysis, DSA).

At the present time, we are emphasizing studies on the geographical extent and physical conditions of the mobilization and migration of rare earth elements and uranium through microcracks in granitic rocks. In core from the Redstone Quarry (New Hampshire) uranium is present in sealed microcracks throughout 3000 feet and in altered mafic minerals within 2 cm of the cracks. In cores of the Sherman granite (Wyoming) U and REE's occur in minerals in partially sealed microcracks in cores separated 30 km; the minerals appear to be identical over the distance. In wall rock of the Geevor (tin) Mine in the Cornwall district of southwest England, U occurs in microcracks and was apparently deposited from hydrothermal fluids after the main tin mineralization. In a reconnaissance examination of a few borrowed samples of the granites near Bangor, Maine, we observed that several minerals that typically contain U are present in microcracks. On the basis of these observations, it appears that transport of U in granitic rocks occurs in microcracks and may be controlled largely by the characteristics of the cracks when they are open.

We plan to examine further the microcracks in the granites near Bangor, Maine, for evidence of REE- and U-mobility. John Ferry has shown previously that a widespread hydrothermal system operated in these granites and has estimated total water flux, pressure, and temperature. We plan also to begin work on microcracks (both open and healed) in eastern black shales.

Contractor: UNIVERSITY OF MINNESOTA
Department of Geology and Geophysics
Minneapolis, Minnesota 55455

Contract: DE-AC02-10837

Title: Experimental Formation of Chalk from Calcareous Ooze

Persons in Charge: W. E. Seyfried, Jr., and T. Johnson

Scope of Work

The purpose of this project is to determine what chemical and physical changes occur during the diagenetic transformation of calcareous ooze to chalk.

Chalk comprises a large part of the marine carbonate record and has been found, in the North Sea, to host recoverable quantities of oil. Chalk deposits hold the promise of future oil fields; thus, an understanding of the formation of chalk is essential to understanding and exploiting its capacity to produce oil.

Marine chalks occur in many stages of diagenesis, from plastic to hard, impermeable limestone. The seemingly haphazard interlayering and localized occurrence of different types of chalks affects the extent and productivity of hydrocarbon pools. The question of why the diagenetic stage of contiguous layers is so variable has yet to be answered.

At the University of Minnesota we have developed a hydrothermal reaction system in which we can expose soft calcareous sediment to elevated temperatures and differential pressure. Samples of tropical South Atlantic calcareous ooze containing differing amounts of low-Mg calcite, aragonite, biogenic opal, and detrital silicates are subjected to accelerated diagenetic conditions in the laboratory. The sediment pore fluids are sampled by a constant-head flow-through technique which allows us to monitor changes in both fluid chemistry and permeability over the course of an experiment. Thus, we can observe the interaction of in situ chemical and physical changes during diagenesis.

Recently we formed a very hard and pure chalk. After initial compaction and dewatering, heating caused further compaction and an increase in permeability. Pressure solution and recrystallization of biogenic high-Mg calcite to low-Mg calcite was indicated by a decrease in pore fluid calcium concentration accompanied by a release of strontium and magnesium from the rock to the pore solution.

The uptake and release of such elements as magnesium will be greatly affected by the percentage and types of clays present in the sediment, the initial pore fluid chemistry, and the diagenetic conditions. We shall examine the differences in chalk diagenesis caused by varying clay percentages and pressure-temperature conditions. We hope to be able to associate natural chalk textures and compositions with differing diagenetic conditions and initial compositions. The changes which occur during laboratory diagenesis also indicate what types of changes should occur in reservoir chalks subjected to fluid injection to enhance petroleum recovery.

Contractor: NATIONAL ACADEMY OF SCIENCES/
NATIONAL RESEARCH COUNCIL
Washington, DC 20418

Contract: DE-FG01-82ER12018

Title: I. Studies in Geophysics

Person in Charge: T. M. Usselman

The Geophysics Research Board (GRB) of the National Research Council, National Academy of Sciences, is conducting a series of studies in geophysics dealing with timely scientific and societal aspects of geophysics and the corresponding demand on geophysical knowledge.

The studies include: (1) problem-oriented studies such as demands on geophysical knowledge in connection with climatic variations, fresh water resources, mineral resources, geothermal and other energy sources, natural hazards, and environmental maintenance; and (2) science-oriented studies such as geophysical data, international programs in geophysics, status of developments and opportunities in geophysics, and impact of technology on geophysics. Each study is conducted by a panel selected for the specific purpose. The preliminary findings of each study are presented to the scientific community for comment at a suitable symposium. Two or three studies are expected to be completed each year.

The studies are guided by the Geophysics Study Committee (GSC). Members of the committee are Arthur E. Maxwell (Chairman), Colin Bull, John C. Crowell, Nicholas C. Matalas, J. Murray Mitchell, V. Rama Murthy, Raymond G. Roble, and Ferris Webster; and Thomas M. Usselman, staff officer.

Studies Completed

- ENERGY AND CLIMATE (Roger R. Revelle, panel chairman). Publisher in 1977 (158 pp.).
- ESTUARIES, GEOPHYSICS AND THE ENVIRONMENT (Charles B. Officer, panel chairman). Published in 1977 (127 pp.).
- CLIMATE, CLIMATIC CHANGE, AND WATER SUPPLY (James R. Wallis, panel chairman). Published in 1977 (132 pp.).
- THE UPPER ATMOSPHERE AND MAGNETOSPHERE (Francis S. Johnson, panel chairman). Published in 1977 (169 pp.).
- GEOPHYSICAL PREDICTIONS (Helmut E. Landsberg, panel chairman). Published in 1978 (215 pp.).
- IMPACT OF TECHNOLOGY BN GEOPHYSICS (Homer E. Newell, panel chairman). Published in 1979 (136 pp.).
- CONTINENTAL TECTONICS (B. Clark Burchfiel, Jack E. Oliver and Leon T. Silver, panel co-chairmen). Published in 1980 (197 pp.).
- MINERAL RESOURCES: GENETIC CONSIDERATIONS FOR PRACTICAL APPLICATIONS (Paul B. Barton, Jr., panel chairman). Published in 1981 (119 pp.).
- SCIENTIFIC BASIS OF WATER RESOURCE MANAGEMENT (Myron B. Fiering, panel chairman). Published in May 1982 (127 pp.).
- SOLAR VARIABILITY, WEATHER, AND CLIMATE (John A. Eddy, panel chairman). Published in July 1982 (104 pp.).
- CLIMATE IN EARTH HISTORY (Wolfgang H. Berger and John C. Crowell, panel co-chairmen). Published in December 1982 (198 pp.).
- FUNDAMENTAL RESEARCH ON ESTUARIES (L. Eugene Cronin and Charles B. Officer, panel co-chairmen). In press: expected to be available in Spring 1983.

Studies in Preparation

- Explosive volcanism: Inception, evolution, and hazards (Francis R. Boyd, panel chairman). Publication is expected in 1983.
- Groundwater contamination (John D. Bredehoeft, panel chairman). Publication is expected in 1983.
- Geophysical data and public policy (Michael A. Chinnery, panel chairman). Publication is expected in 1983.
- Atmospheric electrical environment (E. Philip Krider and Raymond G. Roble, panel co-chairmen). Symposium scheduled for May 1983.

Studies Under Active Consideration

- Recent Crustal Movements

Scope of Work

The modular pattern for the Studies in Geophysics was designed to permit selection of the most timely topics to meet the following objectives:

(1) to set forth the current and prospective contributions that the geophysical sciences can make to such concerns of mankind as energy, nonrenewable resources, and the environment;

(2) to provide government officials with technological and scientific evaluations that can serve as a basis to assist in decision making in matters involving geophysical research and knowledge, both in policies and programs;

(3) to provide to the scientific community a basis for judgments with respect to the development of the basic science of geophysics in the broad sense and with respect to the relative importance to society of the developments within various branches of geophysics.

Contractor: NATIONAL ACADEMY OF SCIENCES/
NATIONAL RESEARCH COUNCIL
Washington, DC 20418

Contract: DE-FGOI-82ER12018

Title: II. Committee on Seismology

Person in Charge: J. W. Berg, Jr.

Scope of Work

The Committee on Seismology meets twice a year to discuss current topics of major importance relevant to seismology, to review with government agency personnel, in particular, the actions that have resulted from recommendations of the committee and its panels, and to take actions to assure a healthy science which is in a position to provide maximum benefits to the nation and to society. These activities are directed at fulfilling the fundamental mission of the committee, as follows: to maintain an active surveillance of major trends in seismology and of developments related to seismology in allied scientific and technical fields, to provide special studies for government agencies on appropriate subjects or problems, to maintain cognizance of and to provide advice on international seismological activities, to provide advice to government agencies concerning the operation of U.S. government-supported seismograph networks and data-dissemination facilities, and to coordinate seismological-related activities within the National Research Council, particularly in the fields of earthquake engineering, rock mechanics, geodesy, geodynamics, and geology. Panels are established to conduct ad hoc studies on topics specified by the committee.

Current Activities

A workshop on seismographic networks was held in March 1982, to address problems associated with the global, regional, and national networks. The report is currently in the process of publication and was distributed by July 1, 1983.

A report on data problems in seismology has been written and is being revised. The revised draft was submitted to the Committee on Seismology for discussion at the next meeting on April 14-15, 1983.

The Panel on Seismological Studies of the Continental Lithosphere is revising its report. The subject matter corresponds with the International Program on the Lithosphere.

Contractor: NATIONAL ACADEMY OF SCIENCES/
NATIONAL RESEARCH COUNCIL
Washington, DC 20418

Contract: DE-FGOI-82ER12018

Title: III. U.S. National Committee for Geochemistry

Person in Charge: W. L. Petrie

Scope of Work

The U.S. National Committee for Geochemistry has two major functions: (1) acting as the corporate U.S. member adhering to the International Association of Geochemistry and Cosmochemistry (IAGC), representing the United States in appropriate international organizations and activities concerned with geochemistry, and (2) promoting the advancement of geochemistry in the United States.

The committee includes a member of the IAGC Council living in the United States who acts in an ex officio capacity as a coordinator who works closely with IAGC: George W. Wetherill, of the Carnegie Institution of Washington and the immediate past president of the IAGC, now holds that position. Other U.S. members of the IAGC Council include Ernest E. Angino (University of Kansas), treasurer, and Ivan Barnes (U.S. Geological Survey, Menlo Park, California), councilor.

The committee meets twice a year usually in conjunction with the spring meeting of the American Geophysical Union and the annual fall meeting of the Geological Society of America. In attendance are ex officio and liaison members and liaison representatives from government agencies, including the U.S. Geological Survey, the Department of Energy, and the National Science Foundation. The U.S. National Committee for Geochemistry regularly reviews, coordinates, and takes action in conjunction with IAGC activities and special reports on a wide variety of geochemical topics.

The committee represents both the National Academy of Sciences, which is the U.S. voting corporate member of IAGC, and geochemists of the United States. The committee supports the IAGC and its council with annual dues, active participation in nominations for IAGC and council offices, the nomination of NAS delegations to IAGC general assemblies and council meetings, and organizing and administering travel grant programs to help our ablest young geochemists attend and present their papers at the concurrently convening quadrennial International Geological Congress. The IAGC met in Paris in 1980: the next meeting is scheduled for Moscow in August 1984.

The committee, which informs members of activities and advances in geochemistry, sponsors symposia and scientific meetings and establishes ad hoc subcommittees or panels, as appropriate, to report on timely topics concerning geochemists both in the United States and abroad. For example, the committee interacts with the U. S. Geodynamics Committee via geochemists assigned to report on specific topics of interest, reviews documents related to radioactive-waste disposal, and arranges workshops, such as that entitled "Basic Research in Organic Geochemistry Applied to National Energy Needs," held at the University of South Florida, St. Petersburg, in December 1980 (gratis copies are available from Mr. W. L. Petrie, NAS-NRC 2101 Constitution Ave., Washington, DC 20418). A study entitled the "Future of Geochemistry" is planned as a sequel to "Orientations in Geochemistry" (1973) by the Panel on Orientations for Geochemistry under the chairmanship of R. M. Garrels.

M. L. Crawford is currently organizing a symposium on fluid migrations in the lithosphere. A major international activity was the Fifth International Conference on Geochronology, Cosmochronology, and Isotope Geology, June 27-July 2, 1982, in Nikko National Park, Japan; the chairman of the committee attended this conference.

The Committee's Constitution provides for members' terms that are normally three years in length, with one third expiring at the end of June each year. The current membership for the U. S. National Committee for Geochemistry is as follows: V. Rama Murthy (Chairman), Keith A. Kvenvolden (Vice Chairman), Larry W. Finger, David A. Hewitt, John R. Holloway, Everett A. Jenne, Fred Mackenzie, Jill D. Pasteris, and Peter J. Wyllie. Liaison with three government agencies is conducted through Edward Schreiber, DOE, Benjamin Morgan, III, USGS, and Alan Gaines, NSF.

Contractor: NATIONAL ACADEMY OF SCIENCES/
NATIONAL RESEARCH COUNCIL
Washington, DC 20418

Contract: DE-FG01-82ER12018

Title: IV. U.S. Geodynamics Committee

Person in Charge: P. J. Hart

Scope of Work

The United States Geodynamics Committee (USGC) was established in 1969 to foster and encourage studies of the dynamic history of the earth, with appropriate attention to both basic science and applications. The USGC work is based largely on the recommendations developed by its 16 reporters and their associated groups. In 1976, at the request of the Geophysics Research Board, the USGC began planning U.S. research activities in solid-earth studies in the 1980's. In the years following, the committee devoted a considerable effort to the program, leading to the report, Geodynamics in the 1980's, published in April 1980. This report urges that research emphasize the origin and evolution of continental and oceanic crust, the continent-ocean transition, the relation of mantle dynamics to crustal dynamics, and a geodynamic framework for understanding resource systems and natural hazards.

Members of the committee are John C. Maxwell (chairman), Don L. Anderson, Bruce A. Bolt, Francis R. Boyd, B. Clark Burchfiel, William C. Kelly, David L. Mackenzie, Prank Richter, Jack E. Oliver, and David W. Scholl; and Pembroke J. Hart, staff officer.

The list of topics and respective reporters has been subject to continual review and revision, as appropriate. As of February 1983, the list is as follows:

Fine structure of the crust and upper mantle	J. E. Oliver
Evolution of oceanic lithosphere	J. R. Heirtzler
Large volume experimentation	R. C. Liebermann
Application of isotope geochemistry to geodynamics	R. E. Zartman
Geodynamic modeling	D. L. Turcotte
Drilling for scientific purposes	E. M. Shoemaker
Magnetic problems	C. E. Helsley
Plate boundaries	J. C. Maxwell
Geodynamic data -- users' needs	W. J. Hinze
Geodynamic data — archiving problems	M. A. Chinnery
Lithospheric properties	T. H. Jordan
Comparative planetology	J. W. Head
Continent-ocean geodynamic transects	R. C. Speed
Electrical properties of the asthenosphere	C. S. Cox
Coordination of major geodynamics-related programs	A. R. Palmer
Celebration of Polar Years and IGY; and Geophysics Film Series	C. L. Drake

The results of the work of the USGC and reporters have been issued in annual reports (published or unpublished). Highlights are outlined below.

In 1973, the USGC strongly urged the application of seismic reflection profiling techniques to the structure of the earth's crust and upper mantle. Two years later a consortium of four universities (COCORP) began applying this technique. That group has now completed profiles totalling more than 4000 km. This technique has now become a standard tool in investigating the earth's crust and upper mantle.

The USGC strongly supported efforts to develop a continental scientific drilling program. The work of the USGC reporter led to two workshops (1974 and 1978). The report of the 1978 workshop, Continental Scientific Drilling Program (1979), contained the principal conclusion that, with advance planning, a greater scientific return could be obtained through add-on experiments involving a relatively small increased expenditure to the existing large investment in drilling by government and industry. The 1979 report also recommended that a national Continental Scientific Drilling Program be organized to facilitate the necessary communication and coordination. As a result of the response by federal agencies to the report recommendations, a Continental Scientific Drilling Committee was created in January 1980 under the Geophysics Research Board. The committee actively encourages the development of this drilling program, including add-on investigations in mission-oriented holes and holes dedicated to basic scientific objectives.

The reporter for plate boundaries organized cross sections across ancient plate boundaries. Eighteen such cross sections are in preparation of which sixteen have been published; two are in press.

The USGC places strong emphasis on the importance of the transition zone between continental and oceanic lithosphere. The USGC recommended that a series of transects be prepared to set forth existing geological, geochemical and geophysical data along a series of 25 corridors around the North American coast — from the continental craton across the transition zone to oceanic lithosphere. The project began in 1980. It involves eight working groups and more than one hundred people. The working groups met in April 1982 to exhibit and review the results of their work to date; a public exhibit (poster session) and symposium were held at the meeting of the Geological Society of America in November 1982. Preparation of the maps and cross sections was essentially complete at that time. Publication of the results will begin in 1983.

The USGC has endeavored to address two main issues regarding geodynamic data: the needs of users and archiving problems. The USGC convened a group in the early seventies to develop new sections of the Guide to International Data Exchange through the World Data Centers and collaborated with the Committee on Geophysical Data in preparing the solid-earth section of the CGD report issued in 1979. The two USGC reporters for geodynamic data are actively involved with the current study on geophysical data and public policy and the task of modernizing the international Guide.

The USGC took initiative in the mid-seventies to encourage and assist the production of gravity and magnetic maps of the United States; the effort expanded to include North America. Preparation of these maps was strongly supported by the Society of Exploration Geophysicists and federal agencies. The gravity and magnetic maps for the United States were published in 1982 and were the subject of special symposia on applications at the fall 1982 meeting of SExG. Publication of the maps for North America is expected within the next year.

The reporter for electrical properties of the asthenosphere has worked closely with the international committee for a program of the same title. It is likely that this effort will lead to a specific cooperative program between the United States and Canada.

In 1980, the USGC appointed a reporter and associated working group to ensure coordination among major geodynamics-related programs, especially the Circumpacific Map Project, Consortium for Continental Reflection Profiling (COCORP), Continental Scientific Drilling Program, Continent-Ocean Transects. Early Crustal Evolution, Deep Sea and Continental Margins Drilling, Gravity Anomaly Map for North America, LASE, Magnetic Anomaly Map for North America, Tectonic Map of North America, and the USGS Geological Framework Program. An important result: agreement was reached that the major maps will be published on the same projection and at the same scale.

The International Union of Geodesy and Geophysics and the International Union of Geological Sciences have organized the International Lithosphere Program (an international program of geodynamics for the 1980's as a successor to the Geodynamics Project, which formally ended in December 1979). The full title of the new program is "Dynamics and Evolution of the Lithosphere: The Framework for Earth Resources and the Reduction of Hazards". International guidance is provided by the Interunion Commission on the Lithosphere. The secretariat of that commission is located in the United States; basic support for the practical operations of the secretariat is provided through the USGC. The international program is developing in a manner partly analogous to the new plans of the USGC. In particular, the emphasis has shifted toward the continents and the continent-ocean transition for reasons of scientific and societal relevance, especially in the areas of resources and natural hazards. The USGC will serve as the U. S. counterpart to the Interunion Commission on the Lithosphere.

The USGC organized a workshop on problems of the lithosphere which was held in March, 1982, in Austin, Texas. The workshop focused primarily on areas of scientific controversy in connection with the lithosphere with the expectation that this will provide guidance regarding the most productive areas for research in the coming years. Proceedings of this workshop are expected to be published in 1983.

Future Work of the USGC

1. Identify actions that can be taken in response to recommendations of the reporters.

2. Identify new priority topics to which the committee can react directly or via a reporter.

3. Address actions to be taken in response to the discussions at the workshop on the lithosphere.

4. Address the program of the International Lithosphere Commission what action should the USGC take? Can the USGC provide guidance and recommendations for the Lithosphere Commission?

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Contractor: NATIONAL ACADEMY OF SCIENCES/
NATIONAL RESEARCH COUNCIL
Washington, DC 20418

Contract: DE-FG01-82ER12018

Title: V. Continental Scientific Drilling Committee

Person in Charge: R. S. Andrews

Scope of Work

The Continental Scientific Drilling Committee (CSDC) was established in January 1980 under the Geophysics Research Board of the National Academy of Sciences-National Research Council (NAS-NRC) to implement the recommendations of the report of the July 1978 Workshop on Continental Drilling for Scientific Purposes held at Los Alamos, New Mexico. This report, Continental Scientific Drilling Program, published by the NAS-NRC in 1979, identified a major goal for this program of maximizing the scientific value of current and planned drilling activities of federal agencies and of industry through add-on experiments, and supplementing these efforts with "dedicated" holes drilled for scientific purposes.

Members of the CSDC are the following: Eugene Shoemaker (Chairman), Lawrence Bonham, Lawrence Cathles, William Dolan, Charles Drake, James Eidel, Howard Gould, Bob Greider, John Hermance, Charles Mankin, L. J. Patrick Muffler, Jack Oliver, Elburt Osborn, C. Barry Raleigh, Richard Traeger, and Matt Walton; and Robert Andrews, staff officer.

Scientific objectives for the national continental scientific drilling program are formulated by the panels of the Committee, five of which currently exist: Thermal Regimes; Basement Structures and Deep Continental Basins; Mineral Resources; Drilling, Logging, and Instrument Technology; and Sample Curation and Data Management. The CSDC established three ad hoc task groups to address specific research drilling targets: the Salton Sea Geothermal Field in California, the Valles caldera in New Mexico, and the Creede Mining District in Colorado.

A DEW (Drilling Early Warning) NEWSLETTER was established by the Committee as its mechanism for communicating with the scientific community. This aperiodic newsletter is distributed to approximately 1700 researchers in universities and other academic institutions, industry, government laboratories and geoscience administrators, geoscience societies, and interested foreign scientists. The most important role of the DEW NEWSLETTER is to announce early in the planning stage important opportunities for add-on investigations to drilling activities of government and industry and encourage collaborative efforts to the benefit of all concerned. It also provides information on the Committee's activities and scientific objectives, announces important meetings and publications, and serves as a forum for interested scientists to exchange information related to drilling. Five newsletters have been distributed to date.

In 1980, the CSDC reviewed the scientific plan for add-on investigations to a drilling activity by industry in northern Illinois and issued a report entitled Comments of the Continental Scientific Drilling Committee on the Document "Illinois Deep Hole Project -- Preliminary Plan". The research proposed in this plan has been completed by the investigators, was reported at 1981 annual meetings of the AGU and the GSA, and will be published in a special issue of the AGU's Journal of Geophysical Research.

The Panel on Thermal Regimes has completed a report to CSDC recommending initiation of a new, highly focused scientific drilling program aimed at understanding the roots of hydrothermal systems related to young magmatic intrusions. Primary targets are high level silicic caldera systems of the Valles caldera and the Long Valley-Inyo-Mono region. The importance of the Yellowstone system is discussed in this report; further considerations will be made concerning the viability of this target for the future. The report also recommended making use of add-on investigations wherever possible to further the understanding of the thermal regime of the Salton Trough. It is anticipated that the report will be issued by the CSDC by the Summer of 1983. A discussion of the targets identified by this Panel, as well as those identified by the Panel on Mineral Resources, will be presented at a symposium in May 1983 during the GSA joint Cordilleran-Rocky Mountain Section meeting in Salt Lake City, Utah.

The CSDC learned of an industry drillhole in the Salton Sea Geothermal Field that may provide an opportunity for add-on investigations, including deepening it from its planned total depth of 12,000 ft to about 18,000 ft. The Panel on Thermal Regimes held an open meeting of interested scientists to discuss this opportunity with the principal investigators; the consensus of the group was enthusiastic endorsement of the scientific merit of the plan.

The panel on Mineral Resources presented a report to the CSDC recommending major emphasis on drilling to study stacked hydrothermal mineral deposits in four mining districts: Creede, Red Mountain, Tonopah, and Butte. The report is being reviewed for issuance by CSDC, probably in mid-1983.

The Panel on Sample Curation and Data Management developed a report concerning curation of drilling samples and ancillary data and recommended means for the formation of an initial organization to handle such activities. The impetus for this Panel was based in part on results of a DOE-OBES workshop on core curation at Los Alamos in 1981. The report is presently being reviewed by the CSDC for issuance later in 1983.

The Panel on Basement Structures and Deep Continental Basins has addressed dedicated drilling based on the U. S. Geodynamics Committee Workshop on Problems of the Lithosphere, the COCORP seismic profiling program, and ocean-continent and ocean margin transect projects, as well as other compilations of geological and geophysical data. The Panel proposed a deep research hole in the Appalachians for its highest priority target; it is preparing a report on its findings for the CSDC. The Panel will also hold special information sessions on research drilling at various future sectional meetings of the GSA.

The Panel on Drilling, Logging, and Instrument Technology is developing plans for a workshop in late 1983 on diagnostics and drilling to develop dialogue between scientists and the drilling/logging community. Focus for the workshop will be on scientific measurements required for research drilling projects recommended by the other panels. The Panel is studying the state of the art in slim-hole drilling and logging and will identify advanced technology required to meet scientific needs. The efficacy of turbine drilling in crystalline rocks is also being addressed by the Panel.

Contractor:	NATIONAL ACADEMY OF SCIENCES/ NATIONAL RESEARCH COUNCIL Washington, DC 20418
Contract:	DE-FG01-82ER12018
Title:	VI. Geological Sciences Board
Person in Charge:	J. W. Berg, Jr.

Scope of Work

The fundamental mission of the Geological Sciences Board is to provide a review of research and public activities in the geological sciences, to assess the health of the disciplines, to identify the research opportunities, and to coordinate geological activities in the structure of the National Research Council. This group takes a leading role in helping to establish scientific policy bearing on larger programs in the geological sciences in and on behalf of the United States. A major charge of the Board is to assess and recommend basic geological research and its applications to meet national and societal needs.

The Board maintains an awareness of the national, societal, scientific, and technological demands that geological sciences will be expected to meet in the future and takes actions which help to meet the demands. Such actions are taken using existing National Research Council activities where possible. The functions of the Board will include the following:

1. Identify basic research opportunities and applied research needs.
2. Review new technology and recommend ways by which the geological sciences can best utilize technological advances to provide maximum benefits to society and to the sciences.
3. Assess educational and manpower requirements relating to future national and societal demands on the geological sciences.
4. Provide a mechanism to enhance interrelationships between domestic and international programs, policies, and problems based on the need to recognize that the geological sciences are intrinsically global in nature.
5. Identify and help provide a means for the dissemination of information to governmental policymakers and the general public on the implications of geological data pertinent to many of our major societal problems.
6. Coordinate activities in the geological sciences with other National Research Council groups having related responsibilities.
7. Provide advice to governmental agencies on request and at the initiative of the Board.
8. Initiate tasks that stem from and are relevant to the functions given above. The conduct and completion of specific tasks will be achieved through the use of workshops, the appointment of subunits, and/or any other means deemed appropriate and expeditious.

Current Activities

1. Committee on Geological Mapping (formerly Working Group on Mapping)

The Working Group supported by the Board has been transformed to a committee. The types of maps that are needed by users are being determined by a questionnaire that has been sent to a statistical sample (3 percent of a population estimated at 70,000 users). Separate funding has been sought for committee activities, but supporting services are provided by the core support of the Board. The data base provided by the questionnaire will be analyzed by the committee and a report will be published. The raw data will be made available to other organizations on request.

2. Ad Hoc Committee on Public Education and Information

The ad hoc committee has met twice and will recommend to the Board that a committee be established to report on needed improvements in geological education in elementary and secondary schools, primarily.

A workshop may be organized by the committee to identify problems, to compile information, and to make some recommendations pertinent to education in the geological sciences.

3. Working Group on Instrumentation

The working group was formed in October 1981, and members are from the Geological Sciences Board, the American Geophysical Union, the Geological Society of America, and the Mineralogical Society of America. This group investigated the needs for geochemical instrumentation, but it was recognized that the needs for instrumentation are acute in all the geological sciences. An interim report has been submitted to the Board, and the information will be submitted to the involved professional societies. This information will be included in reports of the Board. The working group will be disbanded during this year.

4. Committee on Global and International Geology

A committee has been appointed to study and to report on the role that U.S. scientists can play in helping to meet national, societal, and scientific requirements for international information. The study will include an examination of the policies that control the flow of international information.

5. Geological Sciences Board Workshop (June 1981)

The workshop was supported by core support of the Board. The purpose was to report on the status and outlook for the geological sciences. The report has been condensed and is in the process of preparation for publication.

The following committees are funded separately from core support of the Board:

6. Committee on Opportunities for Research in the Geological Sciences

The Board was requested by the Director of the Division of Earth Sciences, National Science Foundation, to prepare a report on the state of the science and to recommend policy for the decade of the 1980s relevant to the academic community and the National Science Foundation. A committee was appointed which has met twice. An interim report was submitted to NSF in November 1982 and a final report has been drafted. It will be submitted to NSF in July 1983.

7. Committee Advisory to the U.S. Geological Survey

   A committee has been appointed to provide advice to the Director of the U.S. Geological Survey on the geological programs of that agency.

8. Committee on Seismology, U.S. National Committee for Geochemistry, and Committee on Geodesy.

   These committees are active and reports in seismology and geodesy are in progress.

Products

The standard product is a report. There have been five reports either published during the past year or in press. Two of these reports have been funded by core support of the Board.

1. Geological Aspects of Industrial Waste Disposal, National Academy Press, 1982. (NAS Program Initiation funds and core support.)

2. Geological Research Applicable to Major Scientific and Societal Problems (in preparation).

Three reports have been supported by external funds to committees operating under the purview of the Geological Sciences Board.

3. Fostering Increased Cooperation Between Geological and Materials Sciences, National Academy Press, 1982.

4. Options for Scientific Ocean Drilling, National Academy Press, 1982.

5. Seismographic Networks: Problems and Outlook for the 1980s (in press).

Contractor: UNIVERSITY OF NEVADA
SEISMOLOGICAL LABORATORY
Reno, Nevada 89557-00180

Contract: DE-AS08-82ER12082

Title: Studies of Magma Chambers in the Western Great Basin

Person in Charge: A. Ryall

Scope of Work

This research is in support of the Continental Scientific Drilling Site Assessment Program and is aimed at defining the configuration of the magma chamber in Long Valley caldera, California; characterizing seismicity associated with magma injection in the caldera; searching for evidence of a possible buried cauldron complex in the Adobe Hills area; and supporting complementary investigations by other agencies involved in the Site Assessment Program. Subtasks are described below.

A. Seismic Network Operation

During the last half of 1982 we deployed five additional seismic stations in the southwest part of the Long Valley caldera, in an area where spasmodic tremor has been observed on at least eight occasions. The US Geological Survey has since reinstrumented seven of the caldera stations, and we are redeploying our equipment at sites north of the caldera. Station spacing in the southwest part of the caldera is less than 10 km; north of the caldera it is 15-20 km. This network is sufficient to provide at least ten readings for the location of earthquakes in the Mammoth Lakes area with magnitude ML<1.5.

The University of Nevada has developed and tested a digital seismographic system for remote operation. The digital station is a data acquisition system that provides broadband (0.05-30 Hz), wide dynamic-range (96 dB) digitization of signals from a three-component set of seismometers, and telemeters the data to a central facility where it is continuously recorded. This system has been tested in an experiment in Hot Creek Valley, central Nevada, and one station is operating at a mine-tunnel station south of Reno. A second station will be installed in a mine at Mina and will be used to determine spectral characteristics of seismic signals affected by attenuation in Long Valley caldera.

B. Data Analysis

Routine analysis efforts have provided a detailed picture of earthquake distribution through February 1983 and work is in progress to develop a master-event algorithm that will enable us to reanalyze data collected before the dense network was installed in 1982. A new system is being assembled that will provide for event detection and conversion to digital format of the analog data transmitted to the Reno data facility. This will facilitate analysis of large numbers of earthquakes and will make possible some limited waveform analysis of the network data.

C. Interpretation

1. Geometry of the Magma Chamber

In order to outline the three-dimensional geometry of the Long Valley magma chamber, we are studying propagation effects for more than a hundred small events around the southern caldera boundary and within the caldera. The primary discriminant for paths through magma appears to be anomalously low (2-3 Hz) signal frequencies combined with the lack of an S-wave. Signal characteristics have been tabulated and mapped for a variety of paths through the caldera and a range of event depths. Current efforts are focused on determining the depth to the top of the main magma body in the central part of the caldera and defining the shape of an apparent tongue of magma in the southern ring fracture system. We are also investigating anomalous propagation effects that suggest the presence of magma bodies in areas outside Long Valley caldera.

2. Magma Injection

Earthquakes in one small area just east of the town of Mammoth Lakes have tended to occur as intensive swarms having the appearance of spasmodic tremor observed in volcanic regions. Current research is aimed at explaining the localization of this type of activity in the southwestern part of the caldera and determining the extent to which swarm activity along the southern caldera boundary may represent dike formation. A detailed study is in progress of a major burst of activity that occurred in this area in early January 1983.

3. Focal Mechanisms

In a paper completed for publication, we have concluded that focal mechanisms of earthquakes in the western Great Basin, including the area around Long Valley caldera, vary systematically with depth. Shallow events have strike-slip mechanisms and events at mid-crustal depth have a strong component of normal slip. This variation, taken together with different fault geometries at different depth, is consistent with a process of lithospheric extension involving normal movement on primary faults and the formation of clusters of fissures or dikes due to crustal spreading at shallow depth. We are now reanalyzing regional and worldwide data for several large earthquakes in 1980 to determine whether those events can be explained by a multiple rupture process rather than the fluid injection model recently proposed by US Geological Survey scientists.

Contractor: STATE UNIVERSITY OF NEW YORK
Albany, New York 12222

Contract: DE-AC02-82ER13013

Title: I. Thermal Evolution of Sedimentary Basins

Person in Charge: T. M. Harrison

Scope of Work

This investigation utilizes the ability of the $^{40}Ar/^{39}Ar$ thermochronological approach to resolve the age, temperature, and, in some cases, the duration of thermal events experienced by microcline-bearing sedimentary rocks. We have determined that detrital microcline grains in sedimentary strata preserve a record of thermal events in the temperature range 100°C to ~ 200°C, depending on length of heating and several mineralogical variables.

Having shown the utility of this approach in a study of a basin formed in a compressional environment (southern San Joaquin Valley, California), we intend to turn our attention to the evolution of basins formed in extensional environmental with an eye to testing existing hypotheses of basin development.

Our initial study will focus on the Albuquerque Basin in the Rio Grande Rift. Microcline separates obtained from both deep drill holes and surface samples will be analyzed by the $^{40}Ar/^{39}Ar$ age spectrum approach. Analysis of the coexisting apatites by fission track dating may also prove useful. A field program will relate the samples at depth with the structural history of the basin. This data should allow resolution of the time-temperature history of various portions of the basin providing sufficient information to assess the validity of simple mathematical models of rifting and subsequent subsidence.

A companion study will be directed at learning more about the transport kinetics of Ar in microcline over geological periods. $^{40}Ar/^{39}Ar$ analyses of microcline separates from the Fenton Hill deep drill holes will further constrain paleo-temperature estimates based on microcline thermochronology.

Contractor: STATE UNIVERSITY OF NEW YORK
Albany, New York 12201

Contract: DE-AC02-81ER0933

Title: II. Crustal Stretching and Subsidence in Sedimentary Basins

Person in Charge: J. F. Dewey

Scope of Work

Stretching and thinning the continental crust is critically important in the maturation, migration, and accumulation of hydrocarbons in and around rifts and sedimentary basins. Isostatic adjustment of the stretched crust/lithosphere leads to rapid synchronous subsidence, providing a basin for sediment accumulation which causes further subsidence. During this stage, the isotherm spacing is reduced by the factor, β, and heat flow increases in both the crust and rapidly accumulating sediment pile, producing conditions under which hydrocarbons mature and begin to migrate into basin flanks. Subsequent to the stretching phase, thermal reequilibration and thickening of the lithosphere are accompanied by an exponentially declining subsidence rate and lessening fault control on thinner sedimentary sequences. During this phase, paleoslopes develop, by differential subsidence, up which hydrocarbons migrate considerable distances into the flanks and adjacent platforms of sedimentary basins.

In such basins as the North Sea, the Pennsylvanian-Permian basins of Texas and Oklahoma, and rifted continental margin basins generally, the stretched continental basement is buried beneath a thick sedimentary sequence and is therefore inaccessible to direct study. Hence, in such basins, the stretching factor, β, must be inferred from the geometry and timing of the sedimentary infill. In some basins, where there is extensive deep well penetration to basement and where the timing of the early parts of the sedimentary infill are known with reasonable precision, the stretching/thermal history may be reconstructed with considerable confidence. Problems arise, however, from unknown or poorly known thicknesses and sedimentation rates in the early rifting phase of many basins. Furthermore, the geometry of and mechanisms by which stretching occurs in such basins are not known. The extent to which mafic dikes play a role in the extension process needs to be known, as well as the geometry of faults in the deeper crust, the relation between shallow fissuring and normal faulting, and the extent and depth of fluid migration during the stretching process.

The Austro-Alpine nappe complex of eastern Switzerland, together with the southern Alps, represents the thinned continental crust of the southern margin of the Alpine trough whose demise led to the growth of the Alps. Both the continental basement and the cover are exceedingly well exposed in eastern Switzerland. By detailed and systematic structural mapping in parts of the Austro-Alpine Nappes, it will be possible to reconstruct, with great precision, the stretching factor, β, and its variability across the basin margin from which the subsidence and thermal history of a large rift complex can be deduced. From the results of this analysis it will be possible to derive a basic picture of the mechanical behavior of the stretched crust-lithosphere during the attenuation process and a knowledge of lithospheric behavior during the prolonged period of Jurassic-Cretaceous cooling. A systematic and very detailed study is also being made of the stratigraphic-structural-thermal maturation history of the intracontinental Pennsylvanian-Permian basins and troughs of Colorado, Texas, and Oklahoma and will be integrated with the Alpine results.

Contractor: STATE UNIVERSITY OF NEW YORK
Department of Earth and Space Sciences
Stony Brook, NY 11794

Contract: DE-AC02-83ER13112

Title: Geochemistry and Origin of Dolomites

Persons in Charge: G. N. Hanson and W. J. Meyers

Scope of Work

The prime objective of this research is to investigate the geochemistry and petrology of regionally extensive dolomites using radiogenic and stable isotopes, trace elements, and a variety of petrographic approaches. We will be applying these approaches to the regionally dolomitized Burlington and Keokuk Formations (Mississippian) in Iowa, Illinois and Missouri. These data will be the basis for testing detailed quantitative geochemical models, including chemical mass transfer models, to constrain the source(s) and migration path(s) of dolomitizing fluids. A general understanding of dolomites is important because they are significant reservoirs for hydrocarbons and in many regions have acted as conduits for migration of petroleum, brines, and ore-forming fluids.

We are using a wide range of high precision major and trace element analyses (Ca, Mg, Fe, Mn, Sr, U, REE) and stable (C, O) and radiogenic isotopes (Sr, Nd, Pb) within a framework of well-established dolomite and calcite cement zonal stratigraphies. In addition, we are investigating fluid inclusions, solid microinclusions, and crystal defect structures in the dolomites. Fluid inclusion work to date has indicated that highly saline fluids and temperatures of 100°C and greater may have been involved in dolomitization. Preliminary solid inclusion work has identified calcite and iron sulfides within the dolomites. Research on major and trace elements has shown that there are at least two major dolomite types which differ from one another in stoichiometry, Fe and Mn. The REE data for the dolomites show that non-carbonate components have a major effect on bulk samples and on acid soluble portions. This indicates that dolomite, or diagenetic calcite, must be physically separated from non-carbonates in order to analyze the REE within the carbonate lattice. Studies are just beginning on extension of the zonal stratigraphies and geochemistry from Iowa southward into Missouri and eastward into Illinois.

These studies have the potential of developing an integrated approach that could be widely applied to fluid-rock systems, not only for studies of dolomitization, but also for cementation of carbonates and sandstones, for migration of elements related to waste disposal and for the chemical evolution of ore fluids.

Contractor: RENSSELAER POLYTECHNIC INSTITUTE
Department of Geology
Troy, New York 12181

Contract: DE-AC0Z-81ER10921

Title: Deep-Burial Diagenesis in Carbonates

Person in charge: G. M. Friedman

Scope of Work

This research program emphasizes the effects of deep burial on creation and elimination of porosity with depth and on changes in textures of carbonate rocks. Two parallel lines of investigation have been employed: (1) experimental compaction tests at various temperatures, pressures and interstitial fluid compositions on natural carbonate sediments and (2) petrographic and mechanical-log analysis of carbonate rocks from boreholes of some of the world's deepest carbonate hydrocarbon (gas) reservoirs.

In the experimental compaction tests we have obtained a breakthrough: in compacted ooids in the presence of distilled water neomorphic microspar of calcite pseudomorphically replaced aragonite, with survival in places, in the ooids of parts of their original fabric. Most of the ooids, replaced neomorphically, retained concentric rims however.

Ooids and skeletal particles compressed at 150°, 200° and 250°C and at 1.5 and 2.4 kilobars, consistent with burial depth of 6 and 9 km, showed appreciable volume reduction. Skeletal particles showed greater response to pressures than ooids and coarser particles lost more void space than finer ones. Skeletal particles become parallel oriented and horizontal as a result of compaction. At a burial depth of 6 to 9 km oolitic facies are likely to retain greater porosity than skeletal facies. Compaction of ooids is greater in distilled water than in marine water. Experimentally compacted ooids develop the same kinds of particle breakage as observed in naturally compacted oolite facies: buckled, spalled, crushed, split, and diagonal fractures. Except for crushed and split particles which increase at higher temperatures, other kinds of breakage are unrelated to temperature effects. At higher temperature ooids develop a higher concentration of longitudinal contacts than other kinds of contacts. By contrast skeletal particles give way from concavo-convex to sutured/fused contacts.

Our study of boreholes reveals that among the world's deepest producing hydrocarbon (gas) reservoirs in the Anadarko Basin of Oklahoma porosity in carbonates is chiefly confined to dolomites. Gas is produced from intercrystal and moldic porosity in Hunton (Ordovician to Devonian) strata at a depth of 25,000 feet. Porosity has been calculated from logs; correcting for the presence of ferroan dolomite indicates porosity greater than previously expected. Our corrections lead us to believe that many productive intervals have been missed. Circumstantial stratigraphic evidence suggests ferroan dolomite to form under conditions of deep burial. The smectite-illite transition has been inferred as a source of sufficient Mg and Fe to form ferroan dolomite; temperature may control this transformation.

Contractor: RICE UNIVERSITY
Houston, Texas

Contract: DE-AS05-83ER13124

Title: Structural Evolution of Central Brooks Range, Alaska

Person in charge: H. Ave-Lallemont

Scope of Work

The main objective of this effort deals with the Jurassic/Tertiary structural evolution of the Brooks Range fold-thrust belt. We apply structural and strain analysis to unravel the sequential development of folds and faults and the kinematics of thrusting. The timing and regional age relations are established by paleontologic and $^{40}Ar/^{39}Ar$ dating. This work centers on the deformation of Upper Devonian to Triassic rocks in and adjacent to the Doonerak Window in the central Brooks Range and of Cretaceous rocks in the northern foothills of the Brooks Range. We test the alternative hypotheses that: (1) the thrust belt experienced continuous northerly transport, or that it underwent a complex transport history involving both north and south motions, and; (2) that development of Mesozoic and Tertiary thrusts are the product of two or more discrete tectonic events, or alternatively are the result of continuous deformation over the last 150 m.y. we also will analyze available seismic reflection lines of the Brooks Range and Arctic Slope. The integration of these studies will allow us to construct balanced cross sections, which are critical for paleogeographic reconstructions of northern Alaska and which may yield important constraints for future hydrocarbon exploration in the region.

Another objective of this work is to test the hypothesis the pre-Upper Devonian rocks were involved in mid-Devonian tectonism related to the development of the Innuitian fold-thrust belt of northern Canada. Studies of pre-Upper Devonian rocks in and south of the Doonerak Window and of rocks in the Schist Belt bordering the southern Brooks Range augmented by metamorphic and $^{40}Ar/^{39}Ar$ studies, will not only constrain models for the mid-Devonian tectonic event, but also for the involvement of these rocks in the younger fold and thrust event of the Brooks Range.

A third objective of ophiolitic rocks south of the Schist Belt, both geochemically and structurally, as similar rocks were involved in the thrusting of the western Brooks Range.

Contractor: SOUTH DAKOTA SCHOOL OF MINES AND TECHNOLOGY
Rapid City, South Dakota 57701

Contract: DE-AC01-82ER12050

Title: Thermally Induced Chemical Migration in Carbonate Rocks

Person in Charge: J. J. Papike

Scope of Work

The main objective of this research continues to be to gain a quantitative understanding of the extent and mechanisms of chemical migration in diverse geological media. The prime site for this study has been the Notch Peak locality in Southwest Utah. Some of the important conclusions resulting from this work so far are: (1) The Notch Peak granitic stock is comprised of three concentric sequentially intruded rock types. They were all derived from the same parent (greywacke) by different degrees of partial melting. (2) Maximum temperature near the contact between the quartz monzolite intrusion and the Cambrian sediments was 575-600°C. (3) Mineral compositions and assemblages in the limestones (as opposed to the argillites) show that fluids were buffered by metamorphic reactions, that domains of equilibrium are small, and that the limestones behaved as a closed system during metamorphism. $^{18}O/^{16}O$, $^{13}C/^{12}C$, and D/H ratios have been determined and show that little or no interaction between the limestone and the intrusion has taken place. (4) In contrast to the behavior of the limestones, extreme depletion of $\delta^{18}O$ in the argillites close to the intrusion indicates fluid/rock ratios $\ll 1$ and $X\ (CO_2) = CO_2/(H_2O+CO_2)$ of the fluid approaching 0. (5) The different behavior of the stable isotopes between limestones and argillites indicates that the limestones were impermeable to fluids relative to the argillites. Thus the flow of fluids was confined to the argillite beds and fractures. (6) In the argillites, migration of Na, K, Rb, Ba, Sr, and Cs has taken place over tens of meters. In contrast, there is no detectable migration of REE, V, Cr, Sc, Zr, Hf, and Al.

New, follow-up, analog sites for chemical migration studies are now being considered. Ideally, such sites include a variety of chemical compositions for the heat and trace element source (the igneous intrusion) which, in turn, intrude a variety of country rock types. In addition, the igneous intrusion should be "spiked" with certain elements of interest (e.g., Cs, Rb) that are in low concentrations in the country rock. This allows the chemical migration path to be monitored effectively. The situation described is probably best represented by the intrusion of a variety of granitic pegmatites into diverse country rock types. Five pegmatite/wallrock interaction sites in the Black Hills, South Dakota, have been selected for detailed study. The purpose of selecting these five pegmatites which exhibit contrasting characteristics is to identify and quantitatively define variables in chemical migration. The variables addressed are: (1) composition of solutions, (2) capability of dispensing solutions into the country rocks and (3) partitioning of mobile elements between mineral phases and solutions derived from pegmatites.

This work is being done in collaboration with J. C. Laul (Pacific Northwest Laboratories), who is conducting the INAA and RNAA analyses.

Contractor: STANFORD UNIVERSITY
Stanford, California 94305

Contract: DE-AT03-76ER71045

Title: I. Porosity with Fluids

Person in Charge: A. M. Nur

Scope of Work

The objectives of this project are (1) to advance our basic understanding of porous or cracked rocks with fluids, and (2) apply the results to geophysical exploration, reservoir evaluation and the study of shallow crustal processes. Specific current studies are:

1. Seismic Attenuation Mechanism. Systematic measurements of wave attenuation in rocks vs pore fluid saturation, pore fluid compressibility, pore fluid viscosity, overburden pressure, strain amplitude temperature and frequency have proven that wave induced fluid flow in the pores is the dominant mechanism of attenuation in rocks at shallow crustal conditions. The results have been applied to the interpretation of deep crustal reflection data and to seismic models of overpressure zones.

2. Network models of porous rocks with fluids. We have developed a general framework to describe all the petrophysical properties of rock, and their dependence on overburden pressure, pore pressure and other variables. The models correctly and accurately predict the hydraulic, electrical and elastic properties of a wide range of porous sedimentary rocks. Results suggest that successful models require that the pore space be characterized as flat grains in contact, rather than cracks with various aspect ratio. The results will provide an order of magnitude improvement in well log interpretation and will allow the development of rigorous petrophysical reservoir models.

3. Velocity and attenuation in heavy oil sands. We have measured the velocities and amplitudes of compressional and shear waves in heavy oil sand sample from Canada and Venezuela as a function of pressure and temperature. The results reveal a 25%-50% decrease in velocity and a 6-7 fold decrease in amplitude upon heating to 125°-150°C. These large changes suggest that seismic methods may be useful in monitoring in situ thermal recovery processes, e.g., steam flooding for enhanced oil recovery.

4. Pore pressure in the crust. We have developed a numerical model which incorporates hydraulic diffusivity, pressure solution and solution transfer, rock and pore deformation, and tectonic strain rate. The model is used to estimate the tectonic and mechanical conditions under which a portion of the crust will develop pore pressure greater than hydrostatic, and as great as lithostatic, and the conditions under which it will drain. The results show that a critical factor—the ratio between permeability and pore volume strain rate--control the fate of pore fluids in the shallow and mid crust. The results of this study will be used to guide exploration efforts to determine the distribution of permeability and pore pressure in the crust, which are particularly important for the evaluation of radioactive waste disposal sites.

Contractor: STANFORD UNIVERSITY
Stanford, California 94305

Contract: DE-AT03-82ER12051.000

Title: II. Mechanism of Zeolite Crystallization and Alteration in Silicate Gasses

Persons in Charge: J. G. Liou and R. J. Donahoe

Scope of Work

The importance of zeolites as a mineral group is well documented, both in natural environments and with respect to their utility in a wide variety of commercial applications. Despite their importance geologically and industrially, relatively little is known about the physiochemical properties which control zeolite formation. It is the purpose of this project to investigate physical and chemical controls on the formation of some Na-K synthetic zeolites.

A. Precipitation Experiments

Phillipsites of varying Si/Al ratio, faujasite, and some low-silica zeolites of unknown structure have been synthesized from clear solutions in the system Na_2O-K_2O-Al_2O_3-SiO_2-H_2O-Cl,NO_3. Chemical controls on phillipsite structure, composition, crystallization process, and growth kinetics were studied. These experiments have shown that the composition of synthetic zeolites can be precisely controlled through varying solution composition parameters. Conversely, the composition of zeolites can give information about the solutions from which they formed. This data has application to zeolite synthesis as well as modeling the chemical evolution of diagenetic and low-temperature hydrothermal fluids.

B. Calorimetric Study of Synthetic Zeolites

Low-temperature heat capacities and heats of solution have been determined for three mixed, Na-K synthetic phillipsites of different Si/Al ratios. Through ion exchange in saturated NaCl and KCl solutions, nearly end-member Na- and K-phillipsites are obtained and their thermochemical properties will be measured. In this way, variation of thermochemical properties as a function of both Na-K and Si-Al mixing can be studied, facilitating the application of the data to natural materials.

C. Nuclear Magnetic Resonance Study of Solutions and Zeolites

Solid MAS ^{29}Si and ^{27}Al NMR has been used to investigate the structures of some of the synthetic zeolites. The spectra may help determine the Si-Al order-disorder in the phillipsites and thereby aid in the calculation of free energies of formation from the calorimetric data. High resolution ^{29}Si NMR has been used to study the distribution of aluminosilicate species in solutions from which zeolites precipitate, as a function of solution composition. These observations, together with those from the precipitation experiments, have laid the basic framework for a comprehensive theory of zeolite crystallization.

Contractor: STANFORD UNIVERSITY
Department of Applied Earth Sciences
Stanford, California 94305

Contract: DE-AT03-82ER12018

Title: III. The Hydrothermal Solubility of Uraninite

Persons in charge: G. A. Parks and D. C. Pohl

Scope of work

Uranium dioxide is a major component in many high-level radioactive waste forms which are slated for long-term remote storage in geologic repositories. Prevention of environmental contamination by radionuclides requires careful assessment of the rate, geographic extent and degree of dispersal of radionuclides from breached repositories or waste disposal sites which in turn depends on complex and sophisticated geochemical and mass transport modeling. Solution mining of in situ uranium deposits which also have uranium dioxides as their major ore presents a similar, though inverse problem. The equilibrium solubility of uranium (IV) dioxide (UO_2)in aqueous solution is a function of many factors such as solution composition (pH, ligand concentration, and ionic strength), oxidation-reduction potential, temperature, and to a lesser degree pressure. The limiting concentration of uranium in natural aqueous systems is dependent on the above factors as well as absorption and complex chemical interaction of the solutions with solid components with which the solution comes into contact.

These constraints must be recognized and accounted for in solution transport and fixation models. The thermodynamic data required to compute these models and limiting solubilities of uranium exists for near-surface conditions of low temperature and high oxidation potential but data for higher temperature and pressure conditions is limited both in extent and precision. This is especially true for reduced tetravalent uranium species.

The major thrust of this work is to obtain equilibrium solubility data for stoichiometric UO_2 in the system UO_2-H_2O while varying pH but while maintaining fO_2 conditions at sufficiently low levels to maintain the U(IV) valence state both in the solid and solution. The temperature range of the experiments is from 100 to 400°C at 500 bars total pressure. We will also attempt to investigate the effect of carbonate and chloride ligands on UO_2 solubility under similar conditions. From the data we may be able to extract equilibrium solubility products as well as hydrolysis and complexation constants.

The experimental approach involves reacting spherical uranium dioxide pellets with solution in Dickson-Gordon hydrothermal apparatus which permits solution samples to be withdrawn into gastight containers at ambient P/T conditions of the experiment. Equilibrium is approached both from over-saturated and under-saturated conditions. The UO_2 solid is characterized both before and after each experiment. The oxygen fugacity (redox potential) is controlled in the experimental apparatus by maintaining a fixed partial pressure of hydrogen within the reaction cell. Attempts to monitor in situ pH at ambient P/T conditions of the experiment have not been successful as it has been found to be impossible to maintain stable electrode potentials for the duration of the experiments. Hydrogen ion activity is now measured at 20°C and extrapolated to the P/T conditions of the experiment by computer.

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Contractor: TEXAS A&M UNIVERSITY
Center for Tectonophysics
College Station, Texas 77843

Contract: DE-AS05-79-ER10361

Title: Mechanical and Transport Properties of Rocks

Person in Charge: M. Friedman

Scope of Work

Several energy-related problem areas require a better understanding of the mechanical and transport properties of rocks under confining pressure at high temperature: geothermal-energy exploration and exploitation, safe underground isolation of toxic waste, siting of stable nuclear power plants, continental deep drilling, and earthquake hazards. Our objective continues to be to learn more about these properties in the brittle and semibrittle regimes through experimental and observational studies, the results of which should be applicable to the prediction of the behaviors of rock masses in which heat has been stored naturally or artificially.

A. The Physical Nature of Fracturing at Depth (N.L. Carter)

The effect of the α-β quartz transition on the creep properties of Sioux quartzite and Westerly granite has been determined dry at 200 MPa confining pressure. The effect is profound for both materials with the creep rate at constant stress decreasing appreciably in the β- field, as it does for synthetic quartz. The deformation is semibrittle and entirely within the transient creep regime. Activation energies in the β- field are 16.5 and 16. 1 Kcal/mole for quartzite and granite, respectively, and 38.7 and 35. 7 in the α-field. Transition temperatures are different for the two materials, but the virtually identical creep behavior confirms our earlier contention that quartz controls the creep rate in granite deformed to low strains.

We are also investigating the effect of strain rate on stress at failure of Westerly granite deformed at 100 Mpa confining pressure and temperatures to 500°C. As expected, the strength of the material decreases both with increasing temperature and decreasing strain rate. However, the form of the dependencies and the flow processes have not yet been determined in these transient creep experiments as the data are currently insufficient.

B. Fracture Permeability of Crystalline Rocks as a Function of Temperature, Pressure, and Hydrothermal Alteration (B. Johnson)

The variation of fracture permeability of low-porosity quartzite is being investigated as functions of effective normal stress and of pore-fluid/rock interactions produced under hydrothermal conditions. The latter is of primary concern, with special attention focused on the roles of dissolution and pressure solution.

The elevated-temperature, corrosive fluid permeability system is completed and under initial shakedown testing. During the construction of this system two complementary topics were investigated, namely: (1) experimental study of the evolution of surfaces undergoing dissolution, with specific emphasis on the changes of surface roughness and asperity shape; and (2) an exploratory experiment to assess whether measurable pressure solution could occur in the time constraints typical of our proposed permeability experiments. For (1) we found that dissolution increases surface roughness and is surface reaction controlled. Defects, such as grain boundaries and microcracks or pores are more important than the crystallographic orientation of the grains. For (2) we found ample evidence of pressure solution in a water-saturated monolayer of quartz grains between surfaces of quartzite with SEM for tests at 300°C for 2-3 days under 10 to 15 MPa effective normal stress across the layer.

C. Mechanical Properties of Rocks at High Temperatures and Pressures
(M. Friedman and J. Handin)

Having acquired a good understanding of the deformation of wet and dry intact crystalline rocks under short-term triaxial compression at the conditions of low effective confining pressures (0-200 MPa) but high temperatures (to partial melting, about 1000°C), we turned our attention to the effects of time of loading and of discontinuities like joints.

In an effort to characterize the time-dependent rheology and flow processes (mechanisms of deformation) operative for presupposed semibrittle behavioral conditions we have conducted a series of drained constant stress creep tests on 2 x 4 cm specimens of dry and water-saturated (Pp = 100 MPa) Westerly Granite at 100 MPa effective confining pressure and temperatures of 300°C to in excess of Tm (1000°C).

Available equations of flow and time to failure are used as response models to characterize the experimental data. Data for 600°C and below (the brittle field) are well fit by an equation of the form: $t_{failure} = t_o P^{-\alpha} \exp(E/RT - K\sigma)$, which has been shown to predict the static time for rock. Using this expression, the calculated apparent activation energies for the summed fatigue processes in the quartz field is 7.5 kcal/mole (300°-400°C dry) and 21. 6 kcal/mole (400-600°C, wet, Pp of 100 MPa). Quasi-steady state flow is observed in the β-quartz field (700-800°C) and the flow behavior is described by $\dot{\epsilon} = A\exp(-Q/RT)\sigma^n$ where Q = 68 kcal/mole, n = 2.7, and A=25.2.

The deformation is multimechanistic; microfracturing of apparent extensile and shear origin, glide in quartz and biotite, microfracture healing, dissolution, mineral alteration, incipient and partial melt are mechanisms observed and evaluated as functions of temperature and strain. The bulk specimen deformation is partitioned into that contributed by the individual mineral species in the analysis. The systematic change in micromechanisms observed with increasing temperature is compatible with the origin of the gradational succession of macroscopic deformation modes from a single narrow fault ($T/Tm \leq .5$), to a shear zone ($T/Tm \cong .6$), to multiple shear fractures ($T/Tm \cong .75$), to uniform flow ($T/Tm \geq .9$). These observations are being accompanied by finite element models of polyphase aggregate deformation.

We have completed preliminary studies of the frictional strengths of artificial joints in Westerly granite at confining pressures of 25 to 200 MPa and temperatures of 400° to 800°C. These are to be compared with the strengths of the intact rock to discover under which conditions the bulk strength of the rock mass is likely to be significantly lowered by the presence of pre-existing fractures; that is, where would frictional and intact-rock strengths become about equal?

We tentatively conclude that the jointed rock is substantially the weaker under all these test conditions and hence that the deformation of the rock mass probably cannot be modeled as a continuum at these physical conditions. Our purpose now is to acquire enough experimental data to allow a good estimate of the errors in predicting rock-mass deformations if the influence of joints is neglected.

Contractor: UNIVERSITY OF TEXAS AT AUSTIN
Department of Geological Sciences
Austin, Texas 78712

Contract: DE-AS05-83ER-13119

Title: Investigation of a Fossil Geothermal System, Hamblin-Cleopatra Volcano, Clark County, Nevada

Person in Charge: D. S. Barker

Scope of Work

In the Lake Mead area, southern Nevada, a Miocene high-potassium andesite-dacite stratovolcano has been segmented by strike-slip and normal faults. Erosion and faulting have exposed the entire volcanic succession, a radial dike system, and sedimentary and volcanic rocks predating and postdating the stratovolcano. Geologic mapping on a scale of 1:12,000, completed before this contract began, permits estimates of the proportions of igneous material that formed sills, dikes, lava flows, and reworked debris during growth of the cone. Rock and mineral major-element and trace-element analyses are being used to test models of magmatic differentiation and magma mixing. An unusually complete record of magmatic evolution can be documented.

Mineralogical and chemical changes were imposed on the volcanic and intrusive rocks by convecting groundwater. The exhumed core of hydrothermally altered rocks represents a fossil geothermal system. Alteration increases toward the focus of the radial dike system, and most units can be sampled in fresh as well as in variously altered states; thus the compositional changes induced by alteration can be distinguished from those produced by magmatic processes. Mineralogical and trace-element changes, and variations in isotopic ratios of oxygen, hydrogen, and carbon, will be related to permeability and porosity variations as well as to sample locations, permitting reconstruction of flow patterns and temperature gradients in this geothermal system.

Contractor: UNIVERSITY OF TULSA
Tulsa, Oklahoma 74104

Contract: DE-AS05-79ER10400

Title: Stability of Natural Gas in the Deep Subsurface

Persons in Charge: C. Barker, N. Takaoh and K. A. Kuenhold

Scope of Work

As average well depth continues to increase and drilling rigs with 50,000 ft. capability are built, considerations of methane survival at depth become important. We have continued to investigate the stability of natural gas in the deep subsurface using a combined theoretical and experimental approach. The stability of natural gas in reservoirs of various mineralogies is being calculated using a computer program that finds the minimum free energy in multicomponent (up to 50), multiphase (up to 30) systems for conditions corresponding to temperatures and pressures down to 40,000 ft (12 km). In the last year this program has been restructured and completely rewritten in more modern code. This has optimized the convergence, improved convenience in handling major versus trace components, and provided much better documentation. The calculations show that methane stability varies widely and that reservoir lithology is an important factor influencing natural gas stability. In particular sulfur, or sulfur-bearing minerals such as anhydrite, reduce methane stability and convert it to hydrogen sulfide. However if iron content is high, pyrite forms and the methane may survive. In many deep carbonates methane remains stable but is diluted with thermally-produced carbon dioxide to give a gas composition that would be uneconomical to produce.

Deep rocks containing gases (in either commercial or non-commercial amounts) are being analyzed and the rock mineralogy determined. To avoid the severe problems of contamination and gas loss during sample retrieval, the gas trapped in fluid inclusions in late stage cements is being used. The fluid inclusions are opened by heating in a vacuum system that forms the inlet to a computer-controlled, fast scanning mass spectrometer. When each individual inclusion ruptures, it produces a burst of gas lasting about 0.5 sec. Software recognizes the burst, retains the previous spectrum as background and records the next six spectra at 1 spectra per 75 msec. The compositional data from these six spectra can be extrapolated back to the time of rupture to give the original gas composition. Analyses of gases in up to 200 inclusions have been made in a single heating experiment with a 10 mg sample of carbonate cement. Gas compositions analyzed so far have ranged from dominantly methane to those with major water, carbon dioxide or hydrogen sulfide, while some low-grade metamorphic samples produced a nitrogen-hydrogen mixture. The gas compositions are being compared with those calculated using the thermodynamic program.

Contractor: WOODS HOLE OCEANOGRAPHIC INSTITUTION
Woods Hole, MA 02543

Contract: EG-77-S-02-4392

Title: Organic Geochemistry of Outer Continental Margin and Deep Ocean Sediments

Person in Charge: J. Hunt

Scope of Work:

The overall objective of this program is to examine the processes of hydrocarbon formation and migration in deeply buried sedimentary rocks. Fine grained shale and carbonate well cuttings from three areas are being studied: (1) the North Slope of Alaska, (2) the U. S. Gulf Coast and (3) continental rises and slopes drilled by the International Program of Ocean Drilling. Pattern recognition of kerogen cracking products obtained at various levels of natural maturation is showing significant changes in the kerogen as it generates oil, condensate, or gas. If these patterns are reproducible in different basins, it could lead to the ability to predict more quantitatively the oil, condensate or gas that has been generated from a particular stratigraphic sedimentary sequence.

A photo-ionization detector is being used to identify individual alkenes, aromatics and heterocyclics in kerogen breakdown products as these are giving clues to both the type and maturation state of the kerogens. Also, cryogenic attachments have been added to the capillary GC columns on the pyrolysis apparatus for more definitive identification and quantitation of C_5 through C_8 compounds.

The oil and gas generation windows plus evidences of hydrocarbon migration are being monitored in six wells from the North Slope of Alaska and four wells from the U.S. Gulf Coast. Samples also are being obtained from two wells targeted for 26,000 and 30,000 feet in the Gulf Coast. Vitrinite reflectance data will be available for all of these wells so that we will be able to determine how pyrolysis maturation indicators vary with the more conventional measurements. In addition, we will have enough wells on the Alaskan Slope so that it may be possible to get a rough idea of three-dimensional formation and migration patterns of both gas and oil over a fairly wide region.

In the coming year, the headspace analysis for light hydrocarbons will be modified by changing to a 100 m fused silica glass capillary column. Studies are currently underway to find the proper liquid phase to give as good separation as the standard HHK column in the C_5-C_8 range. The advantages of the fused silica column over HHK are due to its much higher temperature capability (350°C as compared to 50°C for HHK). This would enable the detailed hydrocarbon analyses to extend to a higher range.

It also is planned to equip the pyrolysis apparatus with a CO analyzer for identifying kerogen type. Studies by Chevron scientists have indicated that this technique is more suitable for rapid screening than conventional procedures.

Contractor: WOODWARD-CLYDE CONSULTANTS
Pasadena, California 91104

Contract: DE-AC03-82ER13014

Title: Earthquake Analyses: Long Valley/Mono Crater

Person in Charge: L. J. Burdick

Scope of Work

During the past year, substantial progress has been achieved in the Continental Scientific Drilling Program toward identifying potential geothermal drilling sites in the Mono Craters/Long Valley area. Recent results have shifted interest from the area of recent volcanics (Mono Craters) to the southern moat and resurgent dome area of the Long Valley caldera. However, the present location resolution and constraint on material properties of the inferred magma body beneath this part of the caldera are both limited. The purpose of the program of research discussed here is to apply sophisticated techniques to high-quality seismic data sets and to integrate the results with interpretations of complementary geophysical data sets.

A. Reflected and Converted Phases from the Long Valley Magma Body (L. J. Burdick and W. Savage)

The S-wave screening effect observed by Ryall and Ryall (1982) is constrained to an anomalous path region in the southern Long Valley. Locally recorded data are being used to further resolve the location and nature of the anomalous region. Excellent-quality three-component digital data have been collected (using the January 1983 swarm events) for ray paths crossing the western side of the southern moat. During the summer of 1983, additional data will be recorded from both explosions and earthquakes in conjunction with the planned refraction experiment in Long Valley. These data will be combined with other available records, and polarization filtering will be used to search for secondary S-wave arrivals. Forward models will be developed for S_xS and S-wave screening to interpret the observations in terms of magma bodies.

B. Source Mechanics of the Larger Earthquakes in the Long Valley Region (T. Wallace)

There has been considerable controversy over the exact nature of the earthquake source mechanisms of the largest events in the 1980 Mammoth Lakes sequence, whether they are double couples produced by slip on faults or injection sources best described by compensated linear-vector dipoles (CLVD). The CLVD source model is being evaluated for the 1980 and 1983 Mammoth Lakes earthquakes using synthetic seismograms matched to observed records. A critical analysis of moment tensor inversion will also be carried out. The similarities in source mechanics for the 1941 and 1980-83 events will be studied using relative waveform inversion. The results of these studies should clarify the applicability of the CLVD interpretation and assess the long-term similarity of earthquake sources in the region. The best source models will be used to investigate the sensitivity of teleseismic short-period body waves to the presence of a magma body.

C. Analysis of Local Seismicity Data (K. McNally)

During the January 1983 swarm, close-in recordings were obtained from stations directly above the swarm. These data are being used to refine hypocentral locations and focal mechanisms for selected swarm events. The space-time microearthquake processes will be assessed in comparison with the 1980 sequences, the large-event source models, and the other geophysical data sets available in the region. The stability of the swarm patterns is important in evaluating the tectonic changes that might be associated with the recent seismicity. These results will be used to assess the degree of uncertainty associated with this apparent change.

Contractor: XDATA CORPORATION
6124 N. Chester Avenue
Indianapolis, Indiana 46220

Contract: DE-AC02-82ER12054

Title: Computerized Underground Image Reconstruction

Person in Charge: K. A. Dines

Scope of Work

The general aim of this work is to develop computer-aided imaging techniques for visualizing the subsurface geology. Previous efforts have concentrated on developing the method of geophysical transmission tomographic imaging using cross-borehole electromagnetic measurements. This technology has been successfully refined and implemented for use in the field. The major goal for the current phase of work is to determine the feasibility of extending this technology for imaging by using data obtained from reflected signals. Near-surface acoustic/seismic imaging situations are of greatest interest, where the region can be probed from the surface or a single borehole.

The scope of work encompasses the development of theoretical models and data processing methods. Computer models are being developed for backscattered measurements obtained by arrays of sources and receivers. Image reconstruction methods based on computer-aided reflection tomography will then be applied to the simulated data to obtain images of reflectivity. The approach is applicable to situations where impedance variations in the medium are of primary diagnostic significance.

This effort is aimed at providing imaging techniques for applications such as the characterization and monitoring of nuclear waste isolation sites, monitoring of underground processes, and evaluation of subsurface resources.

Contractor: YALE UNIVERSITY
Department of Geology and Geophysics
P.O. Box 6666
New Haven, Connecticut 06511

Contract: DE-AS02-76ER10455

Title: Opening Mode Crack Growth in Rock

Person in Charge: Robert B. Gordon

Scope of Work

The objective of this research is to develop an understanding of the fracture strength of brittle rock that can be used in the solution of engineering design problems and in the interpretation of fractures observed in the field. The fracture energy for crack initiation and crack propagation in nine different types of rock was measured with a standardized test procedure. The fracture toughness is found to depend primarily on the preexisting microcrack network in the crystalline rocks and is influenced much less by mineralogical makeup and texture. Rock which is relatively free of microcracks (such as quartzite), or in which cracked or porous material is organized in nearly continuous sheets (such as limestone), or which has a very high concentration of microcracks (such as marble), tends to have a low fracture energy. High fracture energy is found when rock contains a microcrack network that permits development of multiple, partially completed, fracture paths.

The experimental results show that fracture energy depends on cracking rate and on chemical environment. It also depends on the distance a crack has run through a given rock. A most important result of the tests is the demonstration that the fracture energy depends on the state of stress in the test specimen. For example, the presence of compressive stress parallel to the crack plane can cause large changes in fracture energy. Hence, the fracture energy (or fracture toughness) is not a true material property that can be tabulated for different kinds of rock; it must be evaluated for the conditions of loading present in any given problem.

The focus of the research is now on determination of the mechanism by which cracking occurs and by which the "process zone" that surrounds a fracture develops. Knowledge of the mechanisms that control fracture in rock is needed if laboratory results are to be applied in the field or in engineering designs. Conditions in the field or in service cannot usually be duplicated in the laboratory, and a basis for extension or extrapolation of the laboratory data is best found in the physical processes that control crack growth.

GEOSCIENCES RESEARCH (AEC/ERDA/DOE)
Historical Summary
(Operating Funds — Thousands)

ON SITE	FY 1969	FY 1970	FY 1971	FY 1972	FY 1973	FY 1974	FY 1975	FY 1976	FY 1977	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983
ANL	$ 0	$ 0	$ 50	$ 50	1051	$ 60	$ 55	$ 60	$ 55	$ 100	$ 140	$ 240	$ 210	$ 250	$ 250
BNL	–	–	–	–	65	41	0	–	–	–	–	–	–	–	–
LANL	0	0	0	0	55	291	630	560	700	910	1,064	1,420	1,650	1,370	1,064
LBL	–	–	–	–	–	256	310	510	620	660	735	965	1,070	1,160	1,405
LLNL	–	–	–	–	–	–	75	130	130	200	630	910	1,000	1,110	1,200
ORNL	160	150	160	140	0	0	80	140	150	160	240	200	200	430	430
PNL	70	100	70	60	100	123	175	305	200	200	400	500	500	530	530
SNL-A	–	–	–	–	–	–	245	500	400	500	500	1,105	1,210	1,540	1,902
On-Site Total	4270	4300	4300	4290	4461	$ 510	$1,500	$2,422	$2,400	$2,700	$4,070	$6,070	$ 6,210	$ 8,491	$ 7,331
Total Off-Site	9483	9000	9410	9370	9219	$ 535	$ 572	$ 542.75	$ 600.3	$1,150.4	$1,004.31	$2,007,000	$ 2,030,530	$ 3,140.71	$ 4,510
TOTAL OPERATING	9753	9000	9710	9660	9700	$1,330	$2,200	$2,964.75	$2,250.3	$3,550.4	$6,073.310	$8,082,030	$ 8,240,530	$ 8,631.71	11,850
TOTAL EQUIPMENT	–	–	–	–	–	–	–	–	–	–	$ 265,000	$ 000,000	$ 923,000	$ 000,000	000
TOTAL GEOSCIENCES	9753	9000	9710	9660	9700	$1,130	$2,200	$3,004.75	$3,250.3	$3,550.4	$6,338,310	$8,042,000	$10,163,530	$10,631.71	12,740

GEOSCIENCES RESEARCH (AEC/ERDA/DOE)
Historical Summary Off-Site
(Operating Funds — Thousands)

Institution	FY 1969	FY 1970	FY 1971	FY 1972	FY 1973	FY 1974	FY 1975	FY 1976	FY 1977	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983
U/Alaska (Akasofu)	$ 21	$ 20	$ 21	$ 25	$ 32	$ 45	$ 41	$ 52.4	$ 70.0	–	$ 65.4	$ 84.3	$ 100.000	$ 113.141	$ 117.000
U/Alaska (Pulpan)	29	40	48	44	0	102	70	31.6	41.0	58.6	112.7	86.8	70	– T	–
U/Alaska (Kienle)	–	–	–	–	–	–	107	–	–	–	–	–	–	–	–
U/Arizona (Hill)	–	–	–	–	–	–	–	–	–	–	–	69.000	86.510	85.541	100.000
U/Arizona (Norton/Sid)	–	–	–	–	–	–	–	–	–	–	–	–	85.000	98.767	48.219(T)
Arizona State (Novotsky)	–	–	–	–	–	–	–	–	–	–	–	34.00	61.530	96.463	125.100
Aspen Institute (Roberts)	–	–	–	–	–	–	–	–	–	47.6	57.2	76.57	–	–	–
Brown U. (Hermance)	–	–	–	–	–	–	–	–	–	–	84.7	140	613.016	100	332.100
Cal Tech (Abrams)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	72.100
U/California (B) (Reynolds)	70	70	61	61	61	60	63	139	127	148	127	167.9	144.00	100	100.000
U/California (B) (Price)	0	35	27	62	–	–	–	–	–	–	–	–	–	–	–
U/California (B) (Holgason)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	200.027
U/California (D) (MacGregor)	–	–	–	–	–	–	–	–	–	71.2	61.4	22.04	–	–	–
U/California (LA) (Knapoff)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
U/California (LA) (Anderson/Wuman)	–	–	–	–	–	–	46	58	41	90	102.3	107	121	NFXT	–
U/California (LA) (Boehler)	–	–	–	–	–	–	–	–	–	–	–	–	46.564	NFX	60.400
U/California (LA) (Kennedy)	60	60	60	60	60	60	60	60	60	60	72	727	–	–	–
Carnegie Mellon (Kohnen)	–	–	–	–	40	201	–	–	–	–	–	–	–	–	–
U Chicago (Anderson)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	372.013
Columbia U (Fairbridge)	–	–	–	–	–	30	707	–	P	–	–	94.000	NFX	27.010	97.630
Columbia U (Bykse/Jacobs)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
Columbia U (Schatz/Engelder)	0	70	70	66	66	122	140	250	240	206	274	211.6	217.553	218.001	227.304
Ft Lewis College (Ellington)	–	–	–	–	–	–	–	65	62.1	76	100	140	100	100.000	280.700
Harvard Univ. (Thompson)	–	–	–	–	–	–	–	2	–	–	–	–	–	–	–
U/Hawaii (Menghnani)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	372.013
Headquarters Services	–	–	–	–	–	–	–	–	–	–	–	–	–	66.100	50.00
Indianapolis Center for Advanced Research (Dinet	–	–	–	–	–	–	–	–	–	–	–	–	–	0.1	1
U/Minnesota (Jahnson/Seyfried)	–	–	–	–	–	–	–	–	–	–	–	66	62.554	T	–
MIT (Grodzins)	–	–	–	–	–	–	–	–	–	–	–	–	66.176	66.700	NFX
MIT (Aki)	170	164	94	60	0	–	–	–	–	–	–	–	–	–	–
MIT (Simmons)	44	207	–	–	–	–	36	100	139	112.0	142	163	100.376	161	160.260
NAS/NRC (Perrin Alaskan Earthquake)	–	–	–	–	–	–	–	100	–	100	100	10	100	100.961	100.0
NAS/NRC (Perrin U.S. National Committee in Geochemistry)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
NAS/NRC (Vacelman Studies in Geophysics)	–	–	–	–	–	–	–	–	–	–	–	–	10.0	71.0	–
NAS/NRC (Berg Committee on Seismology)	1	10	11	4	2	3	4	4	4	–	0	27	29	66	–
NAS/NRC (Berg Geological/Materials Sciences Study)	–	–	–	–	–	–	–	8.0	9	8.0	8.0	8.0	10.200	10.135	–
NAS/NRC (Berg Geological Sciences Board)	–	–	–	–	–	–	–	–	–	–	14.17	–	0.0247	–	–
NAS/NRC (Hart Geodynamics Committee)	–	–	–	–	–	–	–	–	–	–	–	–	–	12.5	–
NAS/NRC (Andrews Continental Scientific Drilling Committee)	–	–	–	–	–	–	–	–	–	–	16	20	39.6	76.00	–
Naval Weapons Support Center (Tanner)	–	–	–	–	–	–	–	–	–	–	–	68	70	63.3	–
U/Nevada (Ryall)	–	–	–	–	–	–	–	0.0	–	–	–	–	–	–	–
NOAA (Donnelly)	–	–	–	–	–	–	–	–	–	–	–	–	–	76	66.760
Univ. of Oregon (Wolf)	–	–	–	–	–	–	–	–	–	0	–	–	–	–	–
Oregon State (Pahlar)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	103.000
U/Pennsylvania (Paul)	10	207	–	–	–	–	–	–	–	–	–	–	–	30.40	–
Pennsylvania State University (Martin)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
Princeton U (Pettibar)	–	–	–	–	–	–	–	–	–	–	–	61.642	65.230	NFX	T
Queens College (CUNY) (Schreiber)	–	–	–	–	–	–	–	33.9	–	–	–	–	–	–	–
Rice U. (Baker)	–	–	–	–	–	–	–	–	–	–	–	–	60	61.3	48.670
Rice University (Ave-Lallemant)	–	–	–	–	–	–	–	–	–	–	–	10.0	–	0.160	–
RPI (Friedman)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	110.777
SMU (Stockwell)	–	–	–	–	–	–	–	–	–	–	–	–	91.000	98.276	140.954
So. Dakota School of Mines (Puplis)	–	–	–	–	–	–	–	–	–	–	–	–	94.39	69.677	–
U/So. Florida (Beckett)	–	–	–	–	–	–	–	–	–	–	–	–	–	67.388	160.334
Stanford U. (Lou)	–	–	–	–	–	–	–	–	–	–	–	–	34.0247	–	–
Stanford U. (Nur/Kovach)	–	–	–	–	–	–	–	–	–	–	–	–	–	20.537	48.334
Stanford U. (Parke)	–	–	–	–	–	–	–	59.0	65	160.0	140.0	140	140	139	160.000
SUNY, Albany (Dewey)	–	–	–	–	–	–	–	–	–	–	–	–	–	67.000	20.000
SUNY, Albany (Harrison)	–	–	–	–	–	–	–	–	–	–	–	–	60.160	–	NFX(T)
SUNY, Stony Brook (Schaeffer)	–	–	–	–	–	–	–	–	–	–	–	–	–	30.21	130.704
SUNY, Stony Brook (Papike)	–	–	–	–	54	017	–	–	–	–	–	–	–	–	–
SUNY, Stony Brook (Hanson/Wyss)	–	–	–	–	–	–	–	–	–	–	68.7	68.1	64.000	T	–
Univ. of Texas at Austin (Barker)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	111.010
Texas A&M (Friedman)	–	–	–	–	–	–	–	–	–	–	–	–	–	–	54.460
U/Tulsa (Barker)	–	–	–	–	–	–	–	–	–	–	62.6	200.400	202.014	200	201.200
USGS (Hess)	–	–	–	–	–	–	–	–	–	–	68.7	NFX	74.000	71.470	74.000
U/Wisconsin (Wang)	–	–	–	–	–	–	–	–	0.1	64	64	–	–	–	–
Woods Hole (Hunt)	–	–	–	–	–	–	–	–	–	–	–	37.30	37.0	–	–
Woodward-Clyde, Pasadena (Cole/Burdick)	–	–	–	–	–	–	–	–	39.5	–	100	140.00	139.001	100	100.000
XDATA (Dinet)	–	–	–	–	–	–	–	–	–	–	–	–	–	99.73	99.611
Yale U (Gordon)	–	–	–	–	–	–	–	–	–	–	–	–	–	97.255	66.617(T)
Yeshiva U (Cameron)	–	–	–	–	–	–	–	–	–	–	49.14	3.6	34.635	35.637	30.350
Off Site Total	41	30	MT	–	–	–	–	–	–	–	–	–	–	–	–
	9480	9985	9419	6376	6310	6836	6472	6845.75	6865.2	61,160.4	61,894.21	62,667.636	63,656.630	63,140.710	(4,810.942

SUBJECT INDEX

GEOLOGY, GEOPHYSICS, AND EARTH DYNAMICS

Large Scale Earth Movements 8, 10, 12, 13, 85, 87, 88, 102
Evolution of Geologic Structures 28, 44, 57, 65, 85, 87, 88, 91
Properties of Earth Materials 6, 12, 13, 17, 20, 21, 24, 48, 50, 63, 71
Rock Flow, Fracture or Failure 12, 19, 46, 47, 49, 53, 66, 69, 70, 96, 97, 105
Continental Scientific Drilling Program (CSDP) 8, 10, 16, 17, 18, 27, 28, 29, 43, 44, 45, 48, 80, 85, 102

GEOCHEMISTRY

Thermochemical Properties of Geologic Materials 2, 5, 12, 14, 25, 32, 47, 55, 60, 67, 89, 90, 94
Static Rock-Water Interactions 6, 23, 25
Organic Geochemistry 11, 15, 24, 101
Geochemical Migration 2, 3, 23, 37, 62, 92, 95, 99

ENERGY RESOURCE RECOGNITION, EVALUATION, AND DEVELOPMENT

Resource Definition and Utilization 8, 13, 100
Reservoir Dynamics and Modeling 5, 7, 11, 21, 59, 66, 69, 70, 93
Magma Energy Resources 6, 17, 43, 48, 56, 64, 68
Information Compilation, Evaluation, and Dissemination 8, 16, 18, 29, 36,37, 72, 74, 75, 77, 82

HYDROLOGIC AND MARINE SCIENCES

Ground Water Hydrology 7, 11, 93
Fresh Water Systems 72
Oceanography 71, 101

SOLAR-TERRESTRIAL--ATMOSPHERIC INTERACTIONS

Magnetospheric Physics and Chemistry 30, 31, 52, 72
Upper Atmosphere Chemistry and Physics 38, 39
Solar Radiation 38, 54
Meteorology and Climatology 72

INDEX OF TECHNICAL CONTRIBUTORS

Ahrens, T. J., California Institute of Technology 59
Akasofu, S. I., University of Alaska 52
Aki, K., Massachusetts Institute of Technology 69
Albright, J. N., Los Alamos National Laboratory 21
Alvarez, L. W., Lawrence Berkeley Laboratory 10
Alvarez, W., Lawrence Berkeley Laboratory 10
Anderson, A. T., Jr., University of Chicago 64
Andrews, R. S., National Academy of Sciences 80
Apps, J. A., Lawrence Berkeley Laboratory 6
Asaro, F., Lawrence Berkeley Laboratory 10
Ave-Lallemont, H., Rice University 91
Baker, D. N., Los Alamos National Laboratory 30, 31
Baldridge, W. S., Los Alamos National Laboratory 27
Barker, C., University of Tulsa 100
Barker, D. S., University of Texas at Austin 99
Bayhurst, G. K., Los Alamos National Laboratory 23
Benjamin, T. M., Los Alamos National Laboratory 23, 25
Berg, J. W., Jr., National Academy of Sciences 74, 82
Berryman, J. G., Lawrence Livermore National Laboratory 13
Bish, D. L., Los Alamos National Laboratory 24
Blacic, J. D., Los Alamos National Laboratory 19
Blair, S. C., Pacific Northwest Laboratories 36, 37
Boehler, R., University of California, Los Angeles 63
Bonner, B. P., Lawrence Livermore National Laboratory 13
Bos, R. J., University of Arizona 54
Burdick, L. J., Woodward-Clyde Consultants 102
Burnham, A. K., Lawrence Livermore National Laboratory 15
Cafasso, F. A., Argonne National Laboratory 2
Carmichael, I. S. E., Lawrence Berkeley Laboratory 6
Carnahan, C. L., Lawrence Berkeley Laboratory 7
Carrigan, C. R., Sandia National Laboratories 43
Carter, N. L., Texas A&M University 96
Charles, R. W., Los Alamos National Laboratory 22, 23, 25
Chin, R. C. Y., Lawrence Livermore National Laboratory 13
Cohen, A. D., Los Alamos National Laboratory 24
Cole, D. R., Oak Ridge National Laboratory 35
Costin, L. S., Sandia National Laboratories 46
Curtis, D. B., Los Alamos National Laboratory 25
Delany, J. M., Lawrence Berkeley Laboratory 10
Dewey, J. R., State University of New York, Albany 87
Dickson, F. W., Oak Ridge National Laboratory 34
Dines, K. A., XData Corporation 104
Donahoe, R. J., Stanford University 94
Drummond, S. E., Oak Ridge National Laboratory 33, 34, 35
Duba, A. G., Lawrence Livermore National Laboratory 13, 17, 20
Dunn, J. C., Sandia National Laboratories 43, 44
Durham, W. B., Lawrence Livermore National Laboratory 12
Eichelberger, J. C., Sandia National Laboratories 44, 45, 47, 48
Emerson, D. O., Lawrence Livermore National Laboratory 18
Engelder, T., Columbia University 66
Feldman, W. C., Los Alamos National Laboratory 30
Foote, H. P. , Pacific Northwest Laboratories 36, 37
Frantz, J. D., Geophysical Laboratory of Washington, DC 35
Fried, S. M., Argonne National Laboratory 3
Friedman, A. M., Argonne National Laboratory 3
Friedman, G. M., Rensselaer Polytechnic Institute 90

Friedman, M., Texas A&M University 96, 97
Gary, S. P., Los Alamos National Laboratory 30
Gerlach, T. M., Sandia National Laboratories 48
Goff, F. E., Los Alamos National Laboratory 28, 29
Goldstein, N. E., Lawrence Berkeley Laboratory 8
Gooley, R., Los Alamos National Laboratory 24
Gordon, R. B., Yale University 105
Handin, J., Texas A&M University 97
Hanson, G. N., State University of New York, Stony Brook 89
Hardee, H. C., Sandia National Laboratories 43, 44
Harrison, T. M., State University of New York, Albany 87
Hart, P. J., National Academy of Sciences 77
Hauksson, E., Columbia University 65
Hayes, D. B., Sandia National Laboratories 47
Heard, H. C., Lawrence Livermore National Laboratory 12
Hedstrom, G. W., Lawrence Livermore National Laboratory 13
Heiken, G. H., Los Alamos National Laboratory 28
Helgeson, H.C., University of California, Berkeley 62
Hermance, J. F., Brown University 56
Herrmann, W., Sandia National Laboratories 43
Hill, H. A., University of Arizona 54
Holcomb, D. J., Sandia National Laboratories 46, 49
Hones, E. W., Jr., Los Alamos National Laboratory 31
Howard, N. W., Lawrence Livermore National Laboratory 16
Hunt, J., Woods Hole Oceanographic Institution 101
Jacob, K., Columbia University 65
Johnson, B., Texas A&M University 96
Johnson, G. K., Argonne National Laboratory 2
Johnson, T., University of Minnesota 71
Kasameyer, P. W., Lawrence Livermore National Laboratory 17, 18
King, M. S., Lawrence Berkeley Laboratory 9
Kleckner, E. W., Pacific Northwest Laboratories 38, 39
Krumhansl, J. L., Sandia National Laboratories 48
Kuenhold, K. A., University of Tulsa 100
Larson, N. R., Pacific Northwest Laboratories 38, 39
Laul, J. C., Pacific Northwest Laboratories 41
Liou, J. G., Stanford University 94
Luth, W. C., Sandia National Laboratories 42, 46, 48, 49
Lytle, R. J., Lawrence Livermore National Laboratory 17
Majer, E. L., Lawrence Berkeley Laboratory 9
Manghnani, M. H., University of Hawaii at Manoa 68
Marshall, W. L., Oak Ridge National Laboratory 35
Marusak, N. L., Los Alamos National Laboratory 29
McEvilly, T. V., Lawrence Berkeley Laboratory 5, 9
McNally, K., Woodward-Clyde Consultants 103
Mesmer, R. E., Oak Ridge National Laboratory 32
Meyers, W. J., State University of New York, Stony Brook 89
Michalsky, J. J., Pacific Northwest Laboratories 38
Michel, H. V., Lawrence Berkeley Laboratory 10
Miller, D. G., Lawrence Livermore National Laboratory 14
Morrison, H. F., Lawrence Berkeley Laboratory 8
Nakanishi, K. K., Lawrence Livermore National Laboratory 13
Naney, M. T., Oak Ridge National Laboratory 32, 33
Narasimhan, T. N., Lawrence Berkeley Laboratory 5
Navrotsky, A., Arizona State University 55
Norton, Denis, University of Arizona 53
Nur, A. M., Stanford University 93
O'Hare, P. A. G., Argonne National Laboratory 2

Olsen, K. H., Los Alamos National Laboratory 28
Palmer, D. A., Oak Ridge National Laboratory 34
Papike, J. J., South Dakota School of Mines and Technology 92
Parks, G. A., Stanford University 95
Patton, H. J., Lawrence Livermore National Laboratory 13
Perrin, R., Los Alamos National Laboratory 25
Petrie, G. M., Pacific Northwest Laboratories 37
Petrie, W. L., National Academy of Sciences 75
Phillips, S. L., Lawrence Berkeley Laboratory 8
Pitzer, K. S., Lawrence Berkeley Laboratory 6
Piwinskii, A. J., Lawrence Livermore National Laboratory 12, 17
Pohl, D. C., Stanford University 95
Rard, J. A., Lawrence Livermore National Laboratory 14
Raymond, R., Jr., Los Alamos National Laboratory 24
Reynolds, J. H., University of California, Berkeley 60
Rogers, P. Z., Los Alamos National Laboratory 23, 25
Rokop, D., Los Alamos National Laboratory 25
Rundle, J. B., Sandia National Laboratories 44, 45, 46
Ryall, A., University of Nevada Seismological Laboratory 85
Ryerson, F. J., Lawrence Livermore National Laboratory 12, 17
Savage, W., Woodward-Clyde Consultants 102
Scholz, C., Columbia University 66
Schreiner, F., Argonne National Laboratory 2
Schuster, G. J., Pacific Northwest Laboratories 38
Seitz, M. G., Argonne National Laboratory 2
Seyfried, W. E., Jr., University of Minnesota 71
Shankland, T. J., Lawrence Livermore National Laboratory 13, 20, 21
Simmons, G., Massachusetts Institute of Technology 70-
Slater, D. W., Pacific Northwest Laboratories 39
Smyth, J. R., Los Alamos National Laboratory 24
Steindler, M. J., Argonne National Laboratory 2
Stockman, H. W., Sandia National Laboratories 50
Stokes, G. M., Pacific Northwest Laboratories 38
Swanson, S. E., University of Alaska 33
Sykes, L., Columbia University 65
Takaoh, N., University of Tulsa 100
Thompson, J. B., Jr., Harvard University 67
Traeger, R. K., Sandia National Laboratories 45
Tsang, C. F., Lawrence Berkeley Laboratory 5, 11
Usselman, T. M., National Academy of Sciences 72
Vaniman, D. T., Los Alamos National Laboratory 27
Vogel, T. A., Michigan State University 17
Wallace, T., Woodward-Clyde Consultants 102
Wawersik, W. R., Sandia National Laboratories 47
Weed, H. C., Lawrence Livermore National Laboratory 12, 17
Weres, O., Lawrence Berkeley Laboratory 11
Wesolowski, D., Oak Ridge National Laboratory 34
Westrich, H. R., Sandia National Laboratories 48
Whetten, J. T., Los Alamos National Laboratory 19, 27
White, A. F., Lawrence Berkeley Laboratory 10
Witherspoon, P. A., Lawrence Berkeley Laboratory 5, 11
Woods, R. O., Sandia National Laboratories 49
Wukelic, G. E., Pacific Northwest Laboratories 36, 37
Younker, J. L., Lawrence Livermore National Laboratory 15
Younker, L. W., Lawrence Livermore National Laboratory 12, 14, 16, 17
Zeuch, D. H., Sandia National Laboratories 47

40-574 O - 85 - 43

J. Advanced Energy Projects (AEP) Subprogram

1. For the period FY 1981 - FY 1985, please provide the funding profile, including operating expenses and capital equipment, for the AEP subprogram. Please show the amount of funding provided to DOE laboratory researchers and to non-DOE researchers.

Answer:

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ADVANCED ENERGY PROJECTS					
OPERATING EXPENSES	$ 6314	$ 7319	$ 8300	$ 9100	$ 10810
CAPITAL EQUIPMENT	300	320	290	310	320
SUBPROGRAM TOTAL	6614	7639	8590	9410	11130
DOE LABORATORY RESEARCHERS	1319	3370	3848	3548	5000
NON-DOE LABORATORY RESEARCHERS	5295	4269	4742	5862	6130

2. For the period FY 1981 - FY 1985, please provide the amount of AEP funding going to industry.

Answer: Please see the table for the requested information.

BASIC ENERGY SCIENCES
ADVANCED ENERGY PROJECTS
INDUSTRY
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC05 ADVANCED ENERGY PROJECTS					
KC0501 EXPLORATORY ENERGY CONCEPTS					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	$ 0	$ 39	$ 0	$ 0	$ 0
BEND RESEARCH INC	22	430	420	135	600
DYNATECH R/D COMPANY	216	227	195	164	200
EIC LABORATORIES	0	0	134	142	100
ENERGY & ENV ENG INC	0	108	0	0	0
ENERGY & MINERALS RESEARCH	111	0	0	0	0
FORD MOTOR CO	329	49	0	0	0
GENERAL ATOMIC CO	241	258	0	0	0
GENERAL TEL ELECTRONICS	228	243	0	0	0
GT DEVICES INC	274	285	298	300	0
MATHEMATICAL SCIENCES NW	255	255	257	250	150
MEMBRANE TECH & RES INC	0	0	84	89	400

	(B/A in thousands) FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
NATIONAL TECH SYSTEMS	218	220	204	200	300
PHYSICS INTERNATIONAL	250	0	494	400	200
POWER CONVERSION TECHNOLOGY	400	0	0	0	0
RADIATION MONITORING DEV	0	117	116	120	100
S.H.E. CORPORATION	0	121	0	0	0
SOLAMAT INC	175	295	208	200	200
SPIRE CORPORATION	46	0	0	0	0
TECHNASSOCIATES INC	- 3	0	0	0	0
WARREN WEIL ASSOCIATES	25	0	0	0	0
WESTINGHOUSE R&D CENTER	0	0	394	400	100
35KC05 ADVANCED ENERGY PROJECTS					
CAPITAL EQUIPMENT					
GENERAL ATOMIC CO	34	17	0	0	0
MATHEMATICAL SCIENCES NW	0	23	0	0	0

3. **For the period FY 1981 - FY 1985, please provide the amount of AEP funding going to universities.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
ADVANCED ENERGY PROJECTS
UNIVERSITIES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
ADVANCED ENERGY PROJECTS					
KC0501 EXPLORATORY ENERGY CONCEPTS					
OPERATING EXPENSES					
CALIF UNIV OF IRVINE	$ 685	$ 0	$ 0	$ 0	$ 0
CALIFORNIA INST OF TECH	0	0	238	200	300
CASE WESTERN RESERVE U	0	0	277	300	300
CHICAGO UNIV OF	199	100	0	0	0
COLUMBIA UNIV	97	0	0	0	0
CORNELL UNIV	213	151	0	0	0
DAYTON UNIVERSITY OF	0	60	0	0	0
GEORGE WASHINGTON UNIV	0	0	294	300	0
ILLINOIS UNIV OF	120	0	413	400	200
MASSACHUSETTS INST TECH	0	417	- 14	20	0
MINNESOTA UNIV OF	0	228	0	0	0
NEW MEXICO UNIV OF	0	0	268	178	400
NORTHEASTERN UNIV	0	0	- 1	0	0
PENNSYLVANIA UNIV OF	505	101	0	0	0
STANFORD LELAND JR UNVR	0	0	- 3	0	0
STANFORD UNIVERSITY-SSRL	0	350	0	0	0

(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
TUFTS UNIV	0	0	0	154	0
VIRGINIA POLYTECHNIC INST	105	0	0	48	0
WASHINGTON UNIV OF	0	175	216	0	300
WAYNE STATE UNIV	157	0	0	0	0

4. **For the period FY 1981 - FY 1985, please provide the amount of AEP funding going to DOE laboratories.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
ADVANCED ENERGY PROJECTS
LABORATORIES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC05 ADVANCED ENERGY PROJECTS					
KC0501 EXPLORATORY ENERGY CONCEPTS					
OPERATING EXPENSES					
ARGONNE NATIONAL LAB	$ 0	$ 0	$ 512	$ 600	$ 700
BROUKHAVEN NATIONAL LAB	406	859	30	662	520
FERMILAB	10	0	- 8	0	0
IDAHO NATIONAL ENG LAB	0	132	694	240	600
LAWRENCE BERKELEY LAB	0	620	400	500	700
LAWRENCE LIVERMORE NAT LAB	50	360	204	150	460
LOS ALAMOS NATIONAL LAB	0	333	1168	819	900
PRINCETON PLASMA PHYSICS LAB	251	266	305	110	300
SANDIA CORP	223	392	110	201	200
SERI	185	128	143	18	300
35KC05 ADVANCED ENERGY PROJECTS					
CAPITAL EQUIPMENT					
BROOKHAVEN NATIONAL LAB	180	158	106	138	100
LAWRENCE BERKELEY LAB	0	10	10	0	0
LAWRENCE LIVERMORE NAT LAB	0	0	30	50	100
LOS ALAMOS NATIONAL LAB	0	12	94	50	100
PRINCETON PLASMA PHYSICS LAB	51	50	20	0	20
SANDIA CORP	0	50	30	10	0
SERI	35	0	0	0	0

5. **How much of the FY 1985 AEP budget request is committed to ongoing projects, and how much will be available for new starts?**

Answer: Two-thirds, or $7.4 million, is committed to ongoing projects, and $3.7 million is committed to new starts for FY 1985.

6. **The budget justification for AEP (Congressional Budget Request, FY 1985, Volume 3, p. 172) notes that "the subprogram will develop, on a modest scale, a new initiative in exploring novel sources of electromagnetic radiation such as optical klystrons, x-ray and gamma-ray lasers and free electron lasers." What level of funding is anticipated for this initiative, who will be the participants, and what will be the funding levels for each?**

Answer: The anticipated funding level for this initiative is about $1.0 million. The participants will be selected from among university, national laboratory and industrial proposers with strongest technical proposals. Several such proposals are presently under review. The anticipated annual funding level will be in the $0.5 million range over a two year period.

7. **Please describe in detail both the muon-catalyzed fusion and quark-catalyzed fusion projects. At what levels are these projects being funded, and who is carrying out the work?**

Answer: The objective of both projects is to explore alternative options to the mainstream approaches to controlled fusion, these being the magnetically confined plasmas and the inertially confined plasmas. In all controlled fusion research the goal is to find a mechanism that would bring two light nuclei, such as deuterons and tritons, sufficiently close to each other for them to fuse, with a concomitant release of energy. Counteracting this process are strong electrostatic forces causing the nuclei to repel each other. In both "traditional" approaches to fusion (magnetically confined and inertially confined) the effect of the electrostatic forces is overcome by providing the to-be-fused-nuclei with a great deal of kinetic energy (i.e., heating deuterium-tritium plasmas to temperatures of millions of degrees) and causing them to collide with each other. In the muon-catalyzed fusion approach, first proposed some 35 years ago by Andrei Sakharov and, independently, by Louis Alvarez, a negatively charged particle called the meson, or muon, would be substituted in place of one of the electrons in a D-T molecule, i.e., a molecule consisting of one atom of deuterium and one of tritium. Such a substitution causes the molecule to shrink to such small dimensions that the two nuclei fuse instantly and the muon can go on to catalyze another reaction. The attraction of this approach is that the fusion reactions occur essentially at room temperatures. Thus, the need to contain extremely hot plasmas would have been eliminated. The uncertainty has to do with the question: How many fusion reactions can a single muon catalyze? These fusion reaction rates, per muon, have been measured for the first time under the present project carried out jointly by researchers at the Idaho National Engineering Laboratory and the Los Alamos National Laboratory. Even though these reaction rates turned out to be much higher than originally predicted, they are, at present, still too low to render this scheme practical: The energy investment needed to erect a muon would not be returned in the energy released in the reactions catalyzed by that muon. However, mechanisms have been identified, and are presently being examined, which might result in higher reaction rates. Thus, the final verdict on the practicability of muon-catalyzed fusion has not yet been rendered. The project is supported at an annual funding level of about $0.7 million.

The quark-catalyzed fusion approach is much more speculative but also, potentially, much more rewarding. If "fractionally charged" atoms could be found, and found in quantities (as some theories postulate), then a heavy, fractionally charged negative "nucleus" could attract a deuteron and a triton forming an "atom". The radius of this atom would be so small that the deuteron and the triton would fuse almost instantly, and the fractionally charged negative particle could go on to catalyze further fusion reactions. Again, the reaction would occur at room temperatures.

The present effort, carried out jointly at Los Alamos and Lawrence Livermore, is aimed at identifying potential sources of fractionally charged particles (believed to be present in some geological formations) and at developing a method of separating them in large quantities. The annual level of support for this work is about $0.6 million.

8. **Please provide a copy of the report of the April 22-23, 1983 Symposium on Novel Sources of Electromagnetic Radiation.**

   Answer: A copy is enclosed.

9. **Please provide a copy of the latest AEP research summaries.**

   Answer: A copy is enclosed.

Summary of
The Symposium on
Novel Sources of Electromagnetic Radiation

J. Bokor, N. Economou, R. Freeman, V. Granatstein, S. Harris, B. Kincaid, J. Madey, T. McIlrath, P. Morton, D. Nagel, R. Pantell, C. Pellegrini, A. Sessler, P. Sprangle, S. Suckewer, H. Winick, and R. Yen

I. General Remarks

1. Background and Scope

The development of novel sources of electromagnetic radiation can be expected to have significant impact in several areas which are of interest to the Department of Energy (DOE). Notwithstanding the excellent sources which are presently available (e.g. lasers, synchrotrons, gyrotron oscillators, etc.), significant voids exist throughout the electromagnetic spectrum form the microwave to the X-ray region, where new sources would have important consequences both for basic science and practical applications.

A survey of some novel sources which are under development or have been proposed is given in Section II. These sources, if developed, could be expected to cover a wide range of wavelengths and would have major impact on areas and instruments such as: heating and characterization of dense plasmas, new generations of particle accelerators, photochemical processing, high resolution spectroscopy, soft X-ray microscopy and holography, x-ray lithography for integrated circuit fabrication, and for the development of new types of analytical instruments for studies of solids and surfaces, e.g. auger microscopy and pico-second time scale photoemission.

We have specifically excluded consideration of lasers, gyrotron oscillators and synchrotron-sources because these have already proven themselves.

Thus their further development, which also offers considerable promise, is already covered by existing programs at DOE and other agencies. In fact the symposium, upon which this report is based, started out with review talks on lasers, gyrotron oscilators, and synchrotron-sources so that they could be used as a standard against which other novel sources could be compared; i.e. in order to determine what characteristics novel sources offer in extended capabilities or in other advantages. (e.g., lower cost). The abstracts of these three talks are given in the Appendix.

2. Funding Organization

A number of federal agencies are supporting work in the development of novel sources and, in fact, one agency even has its activity collected into a program with exactly that name.

Nevertheless, as is true in many different disciplines, we suggest that the DOE continue its support of novel source development. In fact, we believe that the discipline is ripe for support at a greater level than it has received in the past from DOE and we hope that in the future greater funding for this area will be possible. For all of the reasons listed in this brief Summary, we feel that such added support is timely and justified.

Except for the Defense Programs the only DOE program funding research on novel sources of electromagnetic radiation is the Advanced Energy Projects Division of Basic Energy Sciences. However, that program's ability to support such research is hindered by the requirement that the period of support form any given project should not exceed three years. Experience shows that this is much too short a period to allow the development of a very novel concept of a light source to a point of maturity where it might be of interest to a potential user. X-ray lasers may serve as an example.

A highly promising project at Stanford (Harris) has by now been supported by the ONR for five years, and has yet to demonstrate lasing action, but presently shows great promise. The same is true of another, equally promising project at Princeton Plasma Physics Laboratory (Suckewer), following three and a half years of support by Advanced Energy Projects.

It is evident that a void exists in DOE's ability to support sustained efforts in exploring new concepts of sources of electromagnetic radiation. Possible options to remedy the situation include:

(a) for the potentially interested DOE program such as Materials Sciences, Chemical Sciences, Biology Research, Fusion, etc. to introduce into their programmatic charters the responsibility to support advanced research on novel light sources;

(b) for the Division of Advanced Energy Projects to continue service as a DOE focal point for research on novel light sources but to extend its time limitation beyond three years. We want to emphasize that all of the authors support the flexibility in funding of new ideas which has resulted directly from the three year limit imposed by the Division of Advanced Energy Projects. We thus think that option (b) is only viable if it is coupled with no significant reduction in the flexibility of the Division.

(c) for a new and distinctly identifiable program activity to be defined specifically aimed at the development of new light sources. In view of the Division of Advanced Energy Project's interest and experience in supporting such research, that Division might be a natural candidate for assuming management responsibility for such a new program.

II. Examples of Novel Sources

We present, in this section, brief descriptions of eleven candidate novel sources. Of course this compendium is not complete we present these descriptions only to show the range and depth of concepts which are being considered. We want to emphasize that no meaning is to be attached to the order of presentation.

We also want to point out that there will, surely, be good ideas, yet to be invented, which will be deserving of support. We hope that the DOE will have the ability to recognize such contributions and the means available to support their development.

1. Frequency Multiplication for Extreme Ultraviolet Generation

Idea - Nonlinear optical processes provide simple and flexible mechanisms for generating coherent radiation in wavelength regions not otherwise covered by "conventional" laser sources. In such a process, a high power laser beam (or perhaps a combination of laser beams) is focused into an appropriate material. Due to the enormously high electric field strength in the laser focus, the polarizability of the material may become nonlinear. This nonlinearity of the material response can then lead to the optical harmonic generation as well as sum and difference frequency mixing processes. Recently, extremely powerful ultraviolet excimer lasers have been developed which can provide peak powers of several gigawatts in several narrow wavelength bands, i.e. 193 nm, 248 nm, and 308 nm. Using nonlinear optics, these laser sources may be up-converted to the extreme ultraviolet wavelength region below 100 nm, a spectral region in which there presently exist no laser sources.

Potentiality - such sources of extreme ultraviolet radiation have several attractive characteristics. They retain the spatial and temporal coherence properties as well as the pulse structure of the drive lasers. They can also be tunable, since tunable drive lasers can be used. These characteristics make nonlinear optical sources of coherent radiation functionally equivalent to direct laser sources. The availability of this capability in the extreme ultraviolet region opens up a wide range of diverse new possible applications. Just a few examples are high resolution atomic and molecular spectroscopy, holography, diagnostic of high density plasmas, and photoemission studies of solids and surfaces for materials analysis.

Experiments Performed - Using existing visible dye laser technology, and third order nonlinear processes, complete coverage of the 100 nm - 200 nm wavelength region has been achieved. Typical performance characteristics in this region are average fluxes of between 10^9 - 10^{13} photons per second with pulse widths typically 10 sec and with repetition lates of 10 pulses per second, and resolutions of $\lambda/\Delta\lambda = 10^7$. Using existing excimer laser sources, the region below 100 nm is now being accessed. Here, radiation has been produced in a collection of bands, extending down to 35 nm using nonlinearities as high as seventh order. Flux levels in this region are in the range of 10^6 - 10^9 photons per second. Since shorter pulses are generally used (10-30 psec) time. Bandwiths produce limitations give resolutions $\lambda/\Delta\lambda = 10^5$. A key development in the generation of these extremely short wavelengths has been the use of pulsed, supersonic gas jets as nonlinear media to overcome several materials limitations.

Experiments to be done - Several important directions are identifiable based on the present results. Probably the most important parameter which could be improved is the output flux level. In this area, work needs to be done to improve the drive laser technology, as well as work on improving the gas jet characteristics to increase the medium density. These improvements might also lead to the generation of even shorter wavelengths. However, the present flux levels are already sufficient that many experiments can be done to utilize the unique source of radiation. In particular, the short pulse nature of the emission can be used in conjunction with photoemission techniques as a new tool for the study of ultrafast phenomena in solids. Another area in which additional work needs to be done is in developing methods such that continuous tunability could be extended to this spectral region. Were this to be achieved, coherent radiation sources would be available to continuously cover a huge range of the electromagnetic spectrum from ~ 3μm to 30 nm in wavelength.

2. Channeling Radiation

The Concept - Charged particles channeled in crystals, either between planes or along an axis, traverse periodic trajectories with a periodicity that ranges from a few hundred to a few thousand lattice sites. This motion, which is similar to the motion of a particle in a magnetic undulator, results in the emission of relatively narrowband radiation that is linearly polarized, highly directional, tunable, and with an intensity that is more than an order of magnitude higher than bremsstrahlung. Electrons or positrons at MeV energies emit X-rays in the forward direction, and particles with GeV energies emit γ-rays.

Potentiality - There are three potential applications for channeling radiation:

a. To study the channeling phenomenon.

The characteristics of the radiation are affected by the channeling motion, and thereby provides a mechanism for studying this motion. For example, the radiation linewidth for planar and axial-chanelled electrons is a measure of the time between collisions, and the radiation intensity indicates the occupation probabilities for the bound states.

b. To investigate the properties of crystals in which channeling occurs.

The emission spectrum can be used to determine crystalline potentials, with electrons probing the region near an axis or plane, and positrons probing the region between axes or planes. Defects and impurities in crystals are also amenable to investigation by this new tool.

c. As a source of radiation.

Channeling radiation photon energies have ranged from soft X-rays to γ-rays. The emission is in a γ^{-1} cone, linearly polarized, of picosecond duration, tunable and reasonably intense.

Experiments Performed - Experimental work has been performed by the Stanford group at the Lawrence Livermore National Laboratory, at CERN, at the University of Aarhus, at Saclay, at the University of Illinios, with the Sherpukov accelerator in the Soviet Union, and at SLAC. Both electrons and positrons have been used with particle energies from 1.0 MeV to over 20 GeV.

At the low MeV range a Van de Graaff machine was employed, and linear accelerators were used at the higher energies. Silicon, germanium, diamond, lithium fluoride, gold, and nickel targets have produced channeling radiation thus far, for both axial and planar-channeled particles.

Experiments to be done

a. Experiments should be performed at reduced temeratures. For electrons the primary limitation on coherence length for radiation at room temperature results from thermal vibrations of the atoms. At lower temperatures the linewidth should be less and the intensity higher.

b. Channeling radiation should be measured for kiloampere, MeV particle beams. This will provide a means for studying the destruction of crystals due to intense beams on a picosecond time scale. In addition, very high X-ray photon fluxes can be produced in this manner.

c. Defects and impurities in crystals can be investigated. There have been interesting observations of the effects of nitrogen platelets in diamond on channeling emission. Interstitial impurities, such as gold in silicon, should alter radiation from positrons.

d. There are a variety of crystals yet to be studied, which should be considered as sources for channeling radiation. In particular, low Z materials, such as Be and Al, are of interest because scattering of channeled particles varies as Z^2 due to Rutherford scattering. Therefore, low Z crystals will generate narrower lines. Other crystals, such as magnesium fluoride and calcium fluoride in the fluorite structure, have bound electron channeling states that are localized away from the planes of vibrating atoms, and thus should also produce narrow lines.

3.Highly Efficient Free Electron Lasers

Both the successful operation of the "free electron laser" (FEL) by the group at Stanford and the availability of high power electron beams has raised the exciting possibility of the development of high power highly efficient, tunable lasers. The potential uses of such a laser are enormous and research and development of several schemes are currently under study.

For a highly efficient laser it is necessary to either transfer a large fraction of beam energies to the electromagnetic field or to recover a large fraction of the electric energy after the interacton between the electrons and the electromagnetic wave.

Several experiments are now underway to investigate different methods of achieving a highly efficient laser. For example, a group a the University of California in Santa Barbara is studying a scheme where a low energy beam from a Van de Graff would interact with an FEL producing radiation in the far infared. Only a small fraction of the electron beam energy will be transferred to the radiation on each pass through the FEL so that highly efficient energy recovery is necessary. The group has already shown that they can recover 96 percent of the beam energy, albeit for the case where the beam has not interacted with the FEL. They now need to investigate the interacton between the electron beam and the electromagnetic radiation and to further demonstrate energy recovery of the electron beam after passing through the FEL.

Experiments are continuing with both a group at Los Alamos National Laboratory and a group at Mathematical Sciences Northwest-Boeing on the use of a tapered FEL with an electron beam (~ 20 MeV) from an rf linac. Both laboratories have already demonstrated extraction efficiencies of several percent. The Los Alamos group is presently working on an oscillator experiment and in the future has proposed to study the use of a linac structure for energy recovery. The Mathematical Science Northwest-Boeing group is currently studying the development of an rf linac that can meet the specifications necessary for the electron beam to be used in an FEL. This work should continue and hopefully we will soon have results that can be used to help in the future designs.

At Lawrence Livermore National Laboratory a group has been studying the use of a tapered FEL with an electron beam from an induction linac. The large current available from induction linacs is most useful for high gain devices where a high fraction of the beam energy is transferred to the electromagnetic wave. They have started to build an amplifier experiment using the electron beam (5 MeV) from the ETA. Since the experiment has not yet been started no results have been reported, but results on gain measurements should be available soon.

4. Free Electron Lasers for Scientific Research

Thanks to the contribution of the many individuals working in the field, the free electron laser appears to be well understood theoreticlly. In particular it is clear that the performance of these devices will depend both on the design of the FEL, and on the characteristic of the electron accelerators used to drive them.

To satisfy the potential near-term application of the FEL, it is desirable to use existing accelerator technology whenever posible. Review of the requirements and characteristics of the possible FEL's, and their possible applications, indicate a number of candidates for near-term development:

Sub-mm/Far IR FEL's - Straightforward dc accelerator, such as the Van de Graff generator, or compact rf accelerators, such as the microtron, can be used effectively to drive long wavelength tunable, FEL's in the range 50 $\mu < \lambda < 400$ μm. These devices can be configured to produce high average power of short optical pulses, and are expected to make fundamental contributions in solid state physics in the study of magnetic and lattice excitations, 2-d electronic states, superconductivity and non-linear phenomenon. the technical issues for such device include material selections and design development for the FEL resonators. Sub-mm/ far IR FEL's are presently under construction at the University of California at Santa Barbara and Bell Labs.

Medium-Power IR FEL's - Existing pulsed microwave linear accelerators can, in principle, be used to drive tunable FEL's at wavelengths ~ 2 μm at average power levels approaching 100 watts. The peak power anticipated from such devices would permit efficient (~ 10) harmonic generation at wavelengths as short as 0.5 μm. Potential application of such a device include non-linear infrared phenomenon (excited state molecular spectroscopy) and medical research. Technical issues include the optimization of accelerator emittance, and peak length. Medium power linac-based IR FEL's are presumably under construction at the Navel Research Laoratory and Stanford University.

Medium-Power Visible FEL's - Electron storage rings can be used to drive tunable FEL's at wavelengths 0.3 μm $< \lambda <$ 0.7 μm with power of the order of 10 - 100 watts. Applications include spectroscopy of low cross-section or rare atoms and molecules, materials research, and photochemistry.

Issues include development of optimized wiggler designs and development of storage rings with straight sections long enough to accommidate these wigglers. The basic aspect of visible storage ring operation have been studied in an amplifier experiment at Orsay, France, and an oscillator experiment at Brookhaven National Laboratory. A design for an optimized medium-power storage ring FEL has been prepared by Stanford University.

XUV FEL's - The reflecitivity of existing multi-layer X-ray mirror, and the current density of existing storage ring designs, appear adequate to support operation of XUV free electron lasers between 50Å < λ < 200 Å. Issues for these devices include the length of the required straight sections and the optical figure and power rating of the available optics. Plans for XUV storage ring FEL's are being considered by Stanford University.

5. Coherent Extreme Ultra-Violet (XUV) Radiation from Relativistic Electron Beams

There are currently no intense sources of tuneable coherent radiation below 2000Å. It is now possible to generate intense coherent harmonics of conventional lasers in the range of 20 Å to 2000 Å using optically bunched electron beams. Such a source will find immediate application in high resolution XUV and soft X-ray atomic and lolecular spectroscopy, soft x-ray microscopy and holography, and time-resolved energy transfer measurements in solids.

This method of generating coherent radiation in the XUV region of the electromagnetic spectrum uses a relavistic electron beam whose density is modulated at a period corresponding to the radiation period. This modulation is produced by a means of an interaction between the electrons, a laser beam, and an undulating magnetic field. The undulator is such that the wavelength of the spontaneous radiation from an electron transversing it is equal to the laser wavelength. This interaction will generage a denmsity modulation at the laser wavelength and its harmonics. The bunched electron beam then produced coherent radiation in another undulator magnet.

This method of generating coherent radiation using relativistic electron beams is complementary to the Free Electron Laser (FEL). Although the FEL produces high average power, it is limited by optical cavity losses and decreasing gain to wavelengths in the UV visible and IR, at least with present-day electron storage ring facilities. The present device can go to shorter wavelengths (possibly as short as 20 Å), but with reduced average power.

Computer modeling of the operation of this device has shown that conversion efficiencies of the fundamental laser, to the harmonics, of approximately 10^{-6} are possible in the output range of 500 Å, yielding greater than 10^{10} photons per pulse with a rep rate on the order of 10 Hz, with a bandwidth of approximately 1 GHz (transform limited) and diffraction limited emission angles. This represents laser-like intensity and a brightness at least 10^{5} times greater than any competing source.

No experimental work on laser harmonic generation by an optically bunched beam has been performed to date. A proof of principle experiment should be done, and the free electron laser experiment at the Brookhaven National Laboratory provides a good test site for this work. Further development of an optimized system will make possible a tunable XUV coherent light source, and provide information on the ultimate short wavelength limit of the technique. This method of XUV light generation could be integreted into a dedicated storage ring-based XUV laser facility.

6. Quasi-Optical Cyclotron Maser Concept

The quasi-optical cyclotron maser is a promising new concept for the generation of high power coherent radiation in the millimeter and submillimeter regime. The configuration utilizes an open resonator cavity in which a generating electron beam is injected and propagated along an external magnetic field.

Characteristics - This configuration has a number of potentially very attractive features among them are:

i. high power handling capability (> 100 MW, because of the large interaciton volume),

ii. very high frequency operation (millimeter and submillimeter regime),

iii. high operating efficiency (> 40 percent),

iv. natural made selection,

v. operation at low electron beam voltage (10 keV and higher),

vi. moderately insensitive to beam temperature.

The quasi optical cyclotron maser could find applications in the following areas:

i. power sources for high gradient accelerating structures (operating at about $\lambda = 1$ cm),

ii. electron wave accelerators such as the inverse FEL, beat wave accelerator, etc.

Present Experiments - Presently a small scale porrf-of-principle experiment on the quasi-optical maser concept is underway at the Naval Research Laboratory. In this experiment a 70 keV electron beam of about 10A will be employed. The output radiation is expected to be at 115 GHz.

Future Direction of Research - One area of future theoretical and experimental study should be directed at using highly relaticvistic electron beams (> 1 MeV). Electron beams of energies greater than an MeV or so can carry many kiloamperes of current, resulting in far greater output radiation power. Another future research area is the generation of higher cyclotron harmonics, thus increasing the radiation frequency while maintaining reasonable levels of the applied magnetic field.

7. Plasma Sources of Vacuum Ultraviolet and X-Radiation

Multimillion-degree plasmas radiate copious VUV and X-radiation. Such plasmas, studied in basic research, fusion and weapon programs, have great potential as short wavelength radiation sources. The situation is similar to that for synchrotron radiation about 1970. Some applications have been demonstrated, but the engineering and utilization of dedicated sources must yet be done to realize the potential of plasma sources. We shall outline the background, potentiality, present status and needed work to develop unique and reliable plasma sources of VUV and X-radiation.

High temperature plasmas can be produced in two major ways: (a) beam heating, e.g., at laser-focus, atomic injection into tokamaks etc., or (b) discharge heatings, e.g., BRV, PUFF, plasma focus and other z-pinch devices. Devices which produce large plasmas, such as tokamaks, are excluded from consideration because of their low brightness. Dense plasmas, especially laser-heated plasmas and gas PUFF devices have received most attention as short wavelength radiation sources. However, lasers are more versatile and cleaner than discharge sources, and are more controllable and more suitable for general laboratory use. Also, they have multiple uses such as for probing samples as well as producing plasmas. Hence, attention is restricted henceforth to laser-heated plasma radiation sources.

Laser plasmas emit photons ranging from continua through intermediate band to line spectra. Photon energies from below 1 eV to over 100 keV are available, often with considerable control over the spectrum. Laser-plasmas emit into 2π usually, but they still reached peak powers, after monochromaters, which exceed those available from storage rings (up to about 5 keV). The source size is small, typically less than a few mm. Pulse lengths can be as short as 20 nsec and and at least as long as 20 nsec. Repetition rates of over 100 Hz are possible with some presently-available lasers. In short, laser-heated plasmas offer a range of attractive characteristics which can be viewed as complimentary to those of synchrotron radiation. Further, laser-plasma sources which emit, useful X-ray intensities can be set up in small laboratories (~ 500 ft^2) for about $250,000.

Given the above characteristics, many uses of VUV and X-ray emission from laser-heated plasmas have been considered, and many more will be developed. In fact, many of the same uses to which synchrontron radiation is put will be done with laser-plasma radiation when the scientific and technical communities awaken to their potential. To date, vuv and X-radiation from plasmas (of all sources) have been used for atomic spectroscopy, diagnostics (radiography) of plasmas, simulation of nuclear weapons effects, some limited structural analysis of materials, microlithography, X-ray microscopy of biologicals and calibration of instrumentation. None of these uses has been anywhere near fully exploited. Other large areas are untapped, including X-ray-induced chemical reactions, non-linear X-ray optics, short-wavelength radiation processure and sterilization, long-wavelength analysis of the composition and structure of materials (e.g., by small angle scattering), and dynamic loging of shocks and phase transformations. Most of these areas are both scientifically important and also related to technological application. To exploit these possibilities, work must be done in three areas: (a) laser development, (b) plasma optimization and (c) demonstration of applications.

None of the lasers employed to date in this arena have been designed specifically to heat plasmas for short wavelength emissions. It is clearly possible to design multiple-pass glass lasers and high power excimer systems which will efficiently (> 20) produce VUV and X-radiation. Enough is already known about optimum laser characteristics (wavelength, pulse length and shape, mode quality, energy...) to guide the design of the lasers.

Considerable work has already been done regarding optimization/tailoring of radiation from laser heated plasmas. Parametric studies of laser characteristics (0.25 - 10.6 μm, 10 psec - 40 nsec, mJ - 10kJ...), focusing and pure target composition have been performed with rep rates up to 10 Hz. Spectral, spatial and temporal measurements have been made. However much remains to be done. Short-wavelength (excimer) and high power lasers must be used to assess their utility for driving plasma sources. Targets with specific compositions and complex geometries remain to be measured. The quantity, directionality and suppression of target debris must be measured.

In addition to laser development and plasma optimization, work should be done to further develp already demonstrated application and to assess the potential new applications including those listed above. This will be done naturally be interested parties once a laser facility is available as a short wavelength radiation source or the feasibility of laboratory size facilities is clearly enough demonstrated that users will invest in a suitable system.

8. XUV Lasers

Rapidly decreasing spontaneous emission times make it likely that lasers in the XUV and soft X-ray spectral regions will be constructed by first exciting a metastable storage level, and then by using an intense pico-second time scale laser, to transfer to a radiating level.

A particularly promising approach is based on storage in the metastable quartet levels of the alkali-atoms and alkali-like ions. The proto-type example is the $1s2s2p\ ^4P_{5/2}$ level of neutral Li. Since the spins of the three electrons are aligned, either autoionization or radiation requires a spin flip. The atom is therefore metastable against autoionization for 6 u sec. and against radiation for much longer times.

The radiating target level in Li is the $1S\ 2p^2\ ^2P$ level, which to the extent that L and S are good quantum numbers is forbidden to autoionize. The transition $1S\ 2p^2\ ^2P$ - $1S\ 2p^2\ ^2p$ has an oscillator strength f= .14, and an Einstein A coefficient of about 40 p sec. The lower laser level ($1s^2 2p\ ^2P$) may be emptied by photo-ionization with an incident laser used to effect the quartet to doublet transfer.

Research is now underway to ascertain techniques for obtaining large densities of metastable quartets. One promising approach is to use laser produced X-rays to photo-ionize column II metals which are previously prepared in the lowest triplet level.

Much also remains to be learned about the metastability of these levels in the presence of electrons and ions; for example, low large are fine structure changing collisions which result in auto-ionization. Both theoretical and experimental spectroscopic studies of metastable and quasimetastable levels embedded in high lying continuua are of interest.

It appears probable that XUV laser of this type will operate in the 100Å to 1000Å spectral region. Driving laser of 10J to 20J in a 5 n sec-pulse at 1.06u will probably be required to reach threshold. Output per pulse energy and power will probably be in the range of 1 to 10 mJ and 10^6 to 10^8 watts.

9. Experimental Investigation of X-Ray Laser Development in a Confined Plasma Column

This approach to X-ray laser development in a confined plasma column is based upon the phenomena of rapid plasma cooling by radiation losses. This leads to fast recombination and collsional cascade into upper excited levels of hydrogen-like ions (e.g. CVI), while the lower excited levels depopulate rapidly by radiative transitions, thus creating population inversions and gains. Plasma can be created and heated by powerful lasers and confined by solenoidal magnetic fields. In such a way it is possible to obtain a relatively uniform long and thin plasma column, appropriate medium for X-ray laser development.

The experimental set-up consist of a 0.5 -1 kJoule CO_2 laser, 1 meter long solenoidal magnet for maximum magnetic field B = 100 - 150 kGauss, plasma chamber with gas puffing system, solid targets assemblies and vacuum system, diagnostic instruments, especially spectroscopic instruments and data aquisition system. A CO_2 laser was focused onto either a solid target of carbon, or gas target of CO_2, O_2, Ne.

In the first series of experiments the effectiveness of radiation losses for fast cooling of the plasma column was measured. Two 0.5 m air monochrometers (absolute intensity calibrated) and 0.6 m air spectrometer were used for monitoring, respectively, the time evolution and space distribution of CVI emission lines from 7 → 6 (3434Å) 7 (5291Å) transitions. These measurements have shown that radiation cooling can be more efficient than adiabatic cooling and that magnetic field of order of 90 - 100 kGauss can confine highly ionized ions (e.g. CVI, OVI) in a column within a radius r < 1 mm.

Preliminary measurements of line radiation using two vacuum ultraviolet (VUV) spectrometers have shown strong enhancement of CVI 182 Å line intensity emitted in the axial direction (the 182 Å line was measured relative to the CVI 33.7 Å 2 ▸ 1 resonance transition) in comparison to the transverse direction. This enhancement suggested quite high, single pass gain, G = 4, however, further work is needed to confirm this.

In a separate experiment, observation of line radiation of Li-like ions in the VUV spectral region indicated population inversions between levels n = 4 and 3 for ions from CIV to Ne VIII. Estimated average gain for OVI 4f-3d transition (520 Å) was G = 0.1 which suggested a much higher peak gain, although no attempt has been made yet for the optimization of the population inversion for any of these Li-like ions.

In near future experiments on confirmation of the gain on CVI 182 Å line should be done. For this purpose the time evolution of 182 Å and 33.7 Å line intensities should be measured in the axial and the transverse directions. Also in order to further increase enhancement of CVI 182 Å line different targets design and better CO_2 laser focussing will be employed. In Li-like sequence attempt to increase significantly gain G for 4f-3d transition for CIV to Ne VIII ions as well as exploratron of possibilities to create inversion population and gain in Mg X, AL XI and Si XII ions is expected to be done.

10. Novel Gyrotion Configurations (Ultra-High Peak Power Gyro-Klystrons)

Basic Idea Gyrotrons emit coherent microwave radiation at the electron cyclotron frequency. They can typically operate stably in large overmoded structures since the frequency is fixed by the externally applied magnetic field and thus can have much larger power rating than other types of microwave tubes which are usually fundamental mode devices. Much research and development has been done and is currently underway on long pulse or CW gyrotion oscillators at millimeter wavelengths for heating plasmas in magnetic fusion research.

However other DOE requirements for advanced microwave tubes (such as next generation RF accelerators) require amplifiers rather than oscillators and ultra-high peak power in short pulses (.2 - 1 us) rather than CW power. The gyro-klystron amplifier consisting of 2 or more cavities separated by drift spaces should be investigated for this type of application.

Potential Gyro-klystron amplifiers may be capable of producing gigawatt peak power at λ = 10 cm or 25 megawatt peak power at λ = 1 cm. Amplifier gain would be large (e.g. 40dB) and efficiency may be even larger than obtained with gyrotron oscillators (viz 30 percent - 60 percent).

What Experiments Have Been Performed There were some preliminary experiments on gyro-klystrons at the ~100 kw power level a number of years ago; however, efficiency obtained was relatively low. Since that time, as part of the gyrotron oscillator program, large advances have been made in gyrotron electron gun technology, gyrotron cavity design and gyrotron nonlinear analysis; all of these could be exploited to enhance gyro-klystron performance. A recent experiment at National Research Laboratory involving a gyrotron oscillator with 2 coupled cavities gave 54 efficiency and indicated the potential for gyro-klystron improvement. As for the generation of very high peak power, a recent Soviet experiment using a pulse-line accelerator and a cold cathode produced 25 MW in a 50 ns pulse at λ = 7.5 mm; the configuration used was a single cavity gyrotron oscillator.

What Should Be Done Next A design study should be carried out on gyro-klystrons at several frequencies in the range 3 - 30 GHz with pulsed power levels of possible interest in advanced RF accelerators. Techniques for efficiency enhancement developed for the gyrotron oscillators such as magnetic field profiling should be exploited to the fullest. An early gyro-klystron experiment employing a pulse line accelerator and cold cathode should be carried out to test the design predictions.

A study should be made comparing conventional power suuplies and thermionic cathodes with the pulse line accelerator cold cathode option. Finally, an optimized gyro-klystron should be demonstrated with technology and parameters chosen to impact the advanced accelerator requirement.

11. Femtosecond Laser Spectrosopy

Considerable progess has taken place in the generation of ultrashort optical pulses. A steady progression of developments has led to ever shorter optical pulses and subsequent improvements in our ability to resolve fast spectroscopic events.

Recent progress has made the generation of 65 fsec laser pulses possible. (1 fsec = 10^{-15} seconds) Improvement in amplification technique has permitted the amplification of these short pulses to gigawatt power level. These intense short pulses further allow for the genration of 80 fsec white light continuum pulses extending in spectrum from 1900 A to 1.6 um. Pulse compression technique further allows for he generation of 30 fsec optical pulse.

The application of such short optical pulses are diverse covering the field of solid state physics, chemistry and biology. In particular, femtosecond spectroscopy allows for the study of some of the important energy transfer processes in nature.

The application of these measurement techniques to two specific problems will be discussed here. In the first application, femtosecond optical pulses have been used to investigate the photoconductivity of the representative one-dimesional organic polymer polyacteylene. Results reveal the 100fs hopping time of solitions on the polymer chain at room temperature.

The second application involves the investigation of melting dynamics of silicon after intense short laser pulse excitation. Results indicate an energy transfer rate of 1 psec (10^{-12} sec) or less between the photo-excited electron-hole plasma and the crystal lattice.

Femtosecond laser technology is presently at its infancy and has already showed promising results in the understanding of energy transfer processes in nature. Further improvements in laser technology should allow for even shorter pulses generation. Application of femtosecond laser spectroscopy should have substantial contributions to energy related research in the near future.

Advanced Energy Projects
FY 1983 Research Summaries

December 1983

TABLE OF CONTENTS

Program Description..... 1
Summaries of Projects Active in FY 1983..... 5
FY 1983 Program Data..... 28
Investigator Index..... 29
Institutional Index..... 30

OFFICE OF BASIC ENERGY SCIENCES

DIVISION OF ADVANCED ENERGY PROJECTS (AEP)

Program Description

What projects are supported?

This Division supports exploratory research on novel concepts related to energy. The research is usually aimed at establishing the scientific feasibility of a concept and, where appropriate, also at estimating its economic viability. Because projects supported inevitably involve a high degree of risk, an indication of a high potential payoff is required. An immediate, specific application of the concept is not an absolute prerequisite for consideration; thus, for example, proposers of schemes leading to the development of x-ray lasers are not required to justify their proposals by discussing potential applications of such lasers.

The concepts supported are typically at too early a stage of scientific verification to qualify for funding by DOE programs responsible for technology development. Where doubt exists, such programs are consulted, prior to proposal consideration by AEP, in order to establish their possible interest in the project.

Projects not supported

The AEP Division does not support ongoing, evolutionary research. Neither does it support large scale demonstration projects.

Period of support

By design the period of support is finite, generally not exceeding three years. It is expected that, following such a period, the concept will either be at a stage where it can be supported by a technologically appropriate organization or branch of DOE, or else it will be dropped.

Funding levels

The size of a contract in FY '83 varied between $70,000 and $394,000 per annum.

Who can propose?

Unsolicited proposals can be submitted by universities, industrial organizations, nonprofit research institutions or private individuals. Consideration is also given to ideas submitted by scientists working at national laboratories.

Proposal evaluation

Awards are based on the results of an evaluation process which usually involves a review by external reviewers. Regardless of the outcome of the evaluation, proposers receive copies of reviewers' reports.

Questions asked of the reviewers depend on the subject of the proposal. Some typical questions are listed below:

1. Is the proposed concept new? How does it compare with other work in the field?

2. Are there basic flaws in the scientific (technical) arguments underlying the concept?

3. Are the technological requirements of the proposed concept, including material requirements, within the realm of either present or near term future capabilities?

4. Is there anything about the concept which makes its economics manifestly untenable, even under reasonably optimistic assumptions?

5. Is the anticipated benefit to the public high enough to warrant the Government's involvement in the R&D effort?

Preproposals desired

It is suggested that before a formal proposal is prepared, the proposer should submit a brief outline of the proposed work. The outline should provide enough background information to enable a decision as to whether or not the proposed work programmatically fits the mission of AEP.

Proposals

Once a programmatic interest of AEP in the proposed project has been established, a proposal should be submitted along the guidelines specified in DOE/MA-0095, "Guide for the Submission of Unsolicited Proposals." Each proposal must contain:

- A cover page, prepared in a format specified in DOE/MA-0095, Appendix B.

- A 200-300 word abstract, written in plain English, describing the essence of the project in terms understandable to a layman. The abstract should be in a form suitable for inclusion in DOE program presentations.

- A technical discussion of the proposed concept and a description of the proposed work. While the discussion should be kept brief, there is no formal limitation on the number of pages allotted to this section of the proposal. Since it is this section that will form the basis for the evaluations by technical reviewers, the proposer is urged to make certain that all aspects of the proposed project which are relevant to forming a judgment of the project's merits are adequately covered.

- A statement of work specifying all tasks to be performed in the course of the proposed work.

- Description of available facilities.

- Resumes of key personnel.

- Detailed information on any support for the proposed or related work, past, present or anticipated, including proposals submitted, or about to be submitted, to other organizations.

- A cost estimate for the proposed effort.

Further Information

Inquiries should be addressed to:

Dr. Ryszard Gajewski, Director
Division of Advanced Energy Projects
Office of Basic Energy Sciences
ER-16, GTN
Department of Energy
Washington, D.C. 20545

Phone: 301/353-5995

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OFFICE OF BASIC ENERGY SCIENCES

DIVISION OF ADVANCED ENERGY PROJECTS

Summaries of Projects Active in FY 1983

This section contains brief summaries of all projects active in this Division during Fiscal Year 1983 (October 1, 1982-September 30, 1983). The intent of this compilation is to provide a convenient means for quickly acquainting an interested reader with the program in Advanced Energy Projects. More detailed information on research activities in a particular project may be obtained by contacting directly the principal investigator shown below the project title. Some projects will have reached the end of their contract periods by the time this book appears, and will therefore no longer be active. Those cases in which work was completed in FY '83 are indicated by the footnote: *Project completed.

1. THE CONTINUOUS MEMBRANE COLUMN: A LOW ENERGY ALTERNATIVE TO DISTILLATION

BEND RESEARCH, INC.
64550 Research Road
Bend, Oregon 97701-8599

Walter C. Babcock
Membrane Separations Division

Date Started: February 5, 1982

Funding: FY '83 $118,000 for 12 months

Anticipated Duration: 3 years

The objective of this program is to evaluate membrane separation as an energy-efficient alternative to distillation. Three commercially important separations currently performed by distillation are under investigation: isopropanol from water, ethanol from water, and soy bean oil from hexane. Work is under way in the areas of membrane development and assessment of membrane performance in a "continuous column" module configuration. Results thus far have been positive; for example, energy-consumption calculations based on membrane performance in laboratory-scale separations indicate a 44% savings in energy is possible when a hybrid membrane/distillation approach is used in place of distillation alone to to produce a 90 vol % isopropanol-in-water azeotrope.

2. LIQUID MEMBRANES FOR THE PRODUCTION OF OXYGEN-ENRICHED AIR

BEND RESEARCH, INC.
64550 Research Road
Bend, Oregon 8599

Stephen L. Matson

Date Started: April 16, 1979

Funding: FY '83 $302,000 for 12 months

Anticipated Duration: 5 years

The objective of this program is to develop novel liquid membranes for the energy-efficient concentration of oxygen from air. Oxygen-enriched air will find use in a wide range of industrial, chemical, and combustion processes. The liquid membrane consists of a solvent that contains a dissolved oxygen carrier and that is held within the pores of a membrane support. The oxygen carrier selectively transports oxygen across the liquid membrane by the process of facilitated transport, which results in a product gas highly enriched in oxygen. Recent efforts have focused on increasing the flux of oxygen across these membranes by reducing their effective thickness. Work in progress relates to development of membrane modules in regeneration techniques to extend their life.

3. EXTREME ULTRAVIOLET COHERENT RADIATION DEVICE: TRANSVERSE OPTICAL KLYSTRON

BROOKHAVEN NATIONAL LABORATORY*
Upton, New York 11973

C. Pellegrini and A. van Steenbergen
National Synchrotron Light Source

Date Started: September 26, 1983

Funding: FY '83 $115,000

Anticipated Duration: 3 years

This project is for the development of a new radiation source to be incorporated with the VUV storage ring of the National Synchrotron Light Source (NSLS) which will produce coherent, diffraction limited radiation from 500 Å to 2000 Å. Specifically, this radiation source is a Transverse Optical Klystron (TOK) which makes use of a high power laser in the visible region and a broken periodicity undulator structure in conjunction with the circulating electron beam bunches in the VUV storage input ring to produce, with good efficiency, coherent radiation at the harmonics of the input laser.

*Performed in cooperation with BELL LABORATORIES, 600 Mountain Avenue, Murray Hill, New Jersey 07974, Richard R. Freeman and Brian Kincaid co-principal investigators.

4. FREE ELECTRON LASER TEST, NATIONAL SYNCHROTRON LIGHT SOURCE

BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

C. Pellegrini and A. van Steenbergen
National Synchrotron Light Source

Date Started: May 1, 1980

Funding: FY '82 $298,000 for 12 months

Anticipated Duration: 3 1/2 years

The purpose of this program is to develop a free electron laser test module driven by the circulating beam of a storage ring. The program will explore the effect of the free electron laser on the parameters of the storage ring as well as involve the development of a coherent wiggler to provide the appropriate mechanism for electromagnetic radiation amplification due to repeated interactions of the laser field and the transversely oscillating electrons in the undulator (coherent wiggler). It is anticipated that a basic design for a tunable high average power ultraviolet source with a narrow spectral bandwidth may result from these studies.

5. MEQALAC CLUSTER ION FUSION

BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

Lewis Friedman and Alfred Maschke
Chemistry & Accelerator Departments

Date Started: January 15, 1981

Funding: FY '82 $240,000 for 12 months

Anticipated Duration: 3 years

Proof-of-principle experiments are proposed to demonstrate that isotopic hydrogen molecule cluster ions can be prepared and accelerated. The long range goal of these experiments is the utilization of plasmas produced by accelerated cluster ions for the production of thermonuclear reactions. A cluster ion source has been developed which has produced low intensity beams of narrow mass distribution hydrogen clusters with mass to charge ratios as high as 10^4. Research on fundamental processes in this low temperature ion source designed to improve source intensity is in progress. A high precision "optical bench" beam transport system was developed for use with small aperture MEQALACs. High brightness beams of Argon and Xenon were accelerated in quadrupole focused acceleration columns. Laminar flow was observed in a 10 gap electrostatic quadrupole accelerating column and in a 50 quad transport line.

6. HIGH CURRENT BETATRON
FOR A FREE ELECTRON LASER

UNIVERSITY OF CALIFORNIA
Irvine, California 92717

Norman Rostoker and Amnon Fisher
Department of Physics

Date Started: August 1, 1981

Funding: FY '81 $685,000 for 3 years

Anticipated Duration: 3 years

A modified Betatron is being developed that resembles an Astron. Electrons are injected into an elongated magnetic mirror. The Larmor radius is 6 cm; the distance between mirrors is 80 cm. With a field emission injector (50 kV, 1 amp, 150 nsec) about 20 nC have been trapped for about 10 μ sec. The electron trajectories are helical with an axial period of 40 nsec and an azimuthal period of 3 nsec. Rapid data acquisition is facilitated by a 1 Hz repetition rate. The purpose of the experiment is to study injection, trapping, acceleration and extraction in this new configuration. Multiturn injection has been demonstrated with electrostatic and magnetic inflectors. Acceleration to about 1 MeV has been accomplished with an iron powder ferromagnetic core and increasing the field at the beam from about 100 to 1000 gauss while maintaining the Betatron 2:1 condition. Electrons have been extracted with a gate coil for direct measurement of the trapped charge. The injection is very nearly tangential to the cyclic orbit which should produce a high-current low-emittance beam suitable for a free electron laser. Measurements of the emittance of an extracted beam are the next objective.

7. BIOEXTRACTION OF IRON FROM IRON OXIDES:
REDUCTION OF COKE DEMAND IN STEEL
PRODUCTION BY MICROBIAL BENEFICIATION

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

Michael R. Hoffman
Engineering and Applied Science

Date Started: August 15, 1983

Funding: FY '83 $237,000 for 3 years

Anticipated Duration: 3 years

The objective of this project is to investigate the kinetics and mechanisms of the reductive dissolution of iron oxide minerals such as hematite, geothite, lepidocrocite and limonite by various species of iron-reducing bacteria. Kinetic parameters will be obtained from batch and continuous flow reactor studies in which P_O , temperature, P_{CO} , surface area, E_H, pH and carbon source will be primary variables. Mixed-culture systems will be studied to determine the occurrence of bacterial mutualism. In addition to reductive dissolution by iron-reducing bacteria, the kinetics of dissolution of iron (III) from insoluble oxides in the presence of siderophore-producing organisms will be investigated. Finally, the rate of accumulation of hexagonal magnetite by magnetotactic organisms will be determined. Results of this research will indicate the potential of anaerobic, aerobic and microaerophilic iron-metabolizing microorganisms for a variety of industrial and commerical applications.

8. NEW POLYMER ELECTRODES AND CONDUCTORS BASED ON POLY(HYDROQUINONE/QUINONE) OXIDATION/REDUCTION SYSTEMS

CASE WESTERN UNIVERSITY
Cleveland, Ohio 44106

Morton H. Litt
Department of Macromolecular Science

Date Started: September 15, 1983

Funding: FY '83 $277,000 for 14 months

Anticipated Duration: 14 months

This project has the following goals: 1) To synthesize soluble linear fused ring polyaromatic polymers (ladder polymers) which have attached 1,4-hydroxyl groups; 2) To characterize these polymers. The polymer should be a good electrical conductor. It is expected that the hydroxyl groups can be reversibly oxidized and reduced - making this material a good candidate for a very high capacity electrode. High molecular weight polymers will be made into oriented fibers and films and their mechanical properties as well as electrical properties studied. Fiber of these polymers should be like graphite fibers, but should be solution processable.

9. COLLECTIVE ACCELERATION OF IONS USING HIGH CURRENT RELATIVISTIC ELECTRON BEAMS

CORNELL UNIVERSITY
Ithaca, New York 14853

John A. Nation

Date Started: January 1, 1980

Funding: FY '82 $151,000 for 12 months

Anticipated Duration: 3 1/3 years

Experiments have been completed demonstrating the use of slow space charge waves on an electron beam for the collective acceleration of ions. In this demonstration a beat-wave was used to accelerate protons. The wave phase velocity was controlled by slowly varying the period of a rippled magnetic field. Approximately 3×10^{10} protons were accelerated through 1 MeV at an average field strength of about 2 MV/m. Work is continuing on this scheme to optimize and understand the performance of the accelerator in order that its application to ion accelerators can be adequately defined. In addition, extensive measurements have been made showing the non-linear reduction in the phase velocity of space charge waves on an electron beam. This work will continue under different sponsorship and will also be applied to collective ion acceleration.

*Project completed

10. DEVELOPMENT OF A BIOCHEMICAL PROCESS FOR PRODUCTION OF ALCOHOL FUEL FROM PEAT

DYNATECH R/D COMPANY
99 Erie Street
Cambridge, Massachusetts 02139

Donald L. Wise

Date Started: June 1, 1981

Funding: FY '83 $199,000 for 12 months

Anticipated Duration: 3 years

Peat reserves in the United States represent a significant untapped energy source (1400 quads). This program is directed toward development of a wet process for utilization of peat as the feedstock in liquid fuel production. The process requires solubilization and partial oxidation of the peat (processed 8% solids) to produce dissolved aromatics which are suitable substrates for adapted anaerobic bacteria. Fermentation parameters are adjusted so that organic acids are the product which can be removed and concentrated by liquid-liquid extraction. The acid salts of the fermentation products can then be electrolytically oxidized to form mixed olefins. A mixed alcohol product, suitable for blending with gasoline can be produced by hydration of the olefins.

11. CATALYSIS OF DIRECT METHANOL ELECTRO-OXIDATION IN BUFFERED ELECTROLYTES

EIC LABORATORIES, INC.
111 Chapel Street
Newton, Massachusetts 02158

S. Barry Brummer
Battery Division

Date Started: July 15, 1983

Funding: FY '83 $134,000 for 12 months

Anticipated Duration: 3 years

The catalysis of CH_3OH oxidation in aqueous, concentrated $K_2CO_3/KHCO_3$ electrolytes for direct CH_3OH/air fuel cells will be explored. A major goal is the elimination of all noble metal catalysts. In the first year of the project, the properties of the $K_2CO_3/KHCO_3$ electrolyte relevant to fuel cells will be determined. These include concentration-conductance-water vapor pressure-CO_2 pressure relationships and the kinetic buffering capacity of the electrolyte. The coulombic efficiency of the CH_3OH-to-CO_2 conversion will be investigated as well as the kinetics of CH_3OH oxidation on Pt electrodes.

12. INVESTIGATION OF THE EXTRACTION OF HYDROCARBONS FROM SHALE ORE USING SUPERCRITICAL CARBON DIOXIDE

ENERGY & ENVIRONMENTAL ENGINEERING, INC.
675 Massachusetts Avenue
Cambridge, Massachusetts 02139

James H. Porter

Date Started: July 15, 1982

Funding: FY '82 $110,000 for 12 months

Anticipated Duration: 16 months**

Carbon dioxide has demonstrated solvent properties for organic materials at temperatures and pressures near its critical point: 31^{0}C and 72.8 atm. At these conditions, small changes in pressure have large effects on the density and thus the solvent power of CO_2. This project is an experimental investigation of a cycle to extract hydrocarbons from the shale under conditions of high pressure and condense the hydrocarbons out of the CO_2 solvent at conditions of low pressure and temperature. Experiments thus far indicate that it is predominantly the bitumen fraction of the shale which is being extracted. It is anticipated that conditions of higher temperature and CO_2 flow rates will result in higher oil yield from the kerogen fraction of the shale.

**Includes unfunded extension

13.*PHOTOCHEMICAL URANIUM ENRICHMENT IN SOLIDS

GENERAL ATOMIC COMPANY
P. O. Box 81608
San Diego, California 92138

Earl S. Ensberg

Date Started: July 1, 1981

Funding: FY '82 $258,000 for 12 months

Anticipated Duration: 2 years

Experiments at GA Technologies have established the existence of resolvable isotopic shifts in the visible absorption bands of photochemically active uranyl salts at 10 K, established the conditions for achieving two-photon photoreaction at that temperature, and obtained limited but consistent isotope separation. Although the achieved separation was impractically small, this static, high-concentration approach offers many technical advantages as a method of uranium enrichment. The present program is directed to the scientific assessment of the potential process. The ground state absorption spectrum of normal and oxygen isotope labeled materials have been assigned and improved uranium isotope absorption selectivity achieved. Measurement of the excited state absorption spectrum revealed a substantial red shift relative to the ground state absorption. On the basis of this finding a series of two laser, two-color experiments have been carried out leading to characterization of the reaction branching ratio in the higher excited state, revealing the role of an intermediate reaction product, and providing substantially improved uranium isotope separation.

*Project completed

14. FLUID DYNAMIC ENERGY SEPARATION

GEORGE WASHINGTON UNIVERSITY
Washington, D.C. 20052

J.V. Foa
School of Engineering and Applied Science

Date Started: September 15, 1983

Funding: FY '83 $294,000 for 2 years

Anticipated Duration: 2 years

The object of this study, the "energy separator", is a new kind of air conditioning and heating device that promises advantages of energy economy as well as of ruggedness and mechanical simplicity. It has only one moving part, a free-spinning rotor. Air entering it is discharged through slanting orifices on its periphery, causing it to spin. The emerging air separates into hot and cold streams whose difference in temperature can be regulated as desired. The hot output is actually not in the form of heat but rather in the form of recoverable mechanical energy that, if not used for heating, may be utilized to drive a turbine to help the compressor drive, thereby saving energy. Among the energy separator's applications of greatest interest from the standpoint of energy conservation are: (a) those involving the simultaneous heating and cooling of separate spaces; (b) heat pumps; (c) the air conditioning and structural cooling of high-speed vehicles, where the high boundary layer temperature makes it impracticable to dump heat overboard through heat exchangers; (d) industrial processes requiring the "freezing", through extremely rapid cooling, of the high-temperature equilibrium composition of a gas; (e) simultaneous refrigeration, heating, and power generation on board refrigerated ships, and (f) those heating and cooling applications in which mechanical simplicity, low cost, and ruggedness are at a premium.

15. RESEACH AND DEVELOPMENT OF A MASS ACCELERATOR (MAID) AS A DRIVER FOR IMPACT FUSION

GT-DEVICES
5705A General Washington Drive
Alexandria, Virginia 22312

Derek Tidman and Shyke Goldstein

Date Started: May 6, 1981

Funding: FY '83 $297,000 for 12 months

Anticipated Duration: 3 years

The objective of this program is to demonstrate that high pressure plasma jets in the kilobar range can be used to propel solid projectiles to high velocity. The basic concept is to accelerate a solid mass (e.g., 0.5 gram) via a series of momentum kicks provided by sequentially directing the high pressure plasma jets onto the rear projectile surface as it passes through each module. This new approach to mass acceleration has been successfully demonstrated using 10 plasma discharge modules (with projectile sensing and timing circuits) aligned in a manner similar to a linear accelerator. Experiments in which the accelerator has been operated in a sense-and-kick mode have achieved velocities of 4 km/sec and velocities above 6 km/sec are expected in the near future with this small scale demonstration device. The effort is also directed to determining whether a large scale version of such an accelerator could be used as a driver for impact inertial fusion, or other energy related applications such as acquiring a data base for equation-of-state information at high pressures. This system appears to provide a low cost approach to these objectives.

16. MEASUREMENT OF THE EFFICIENCY OF MUON-CATALYZED FUSION

IDAHO NATIONAL ENGINEERING LABORATORY
EG&G Idaho, Inc., P.O. Box 1525
Idaho Falls, Idaho 83415

Steven E. Jones
Scientific Information AGM

Date Started: March 8, 1982

Funding: FY '83 $344,000 for 12 months

Anticipated Duration: 3 years

An experimental investigation of muon-catalyzed fusion in deuterium-tritium mixtures has producted a number of new results. We have measured directly for the first time the high-energy neutron yield of the reaction $\mu^- + d + t \rightarrow \mu^- + He + n + 17.6$ MeV. At high deuterium-tritium densities (up to 60% of liquid hydrogen density), copious 14 MeV neutron production has been observed, demonstrating many d-t fusions per muon. Furthermore, the neutron yield has been shown to increase with the temperature of the deuterium-tritium gas in the range 100K - 550K. The fusion yield also depends on the mixture density and deuterium-tritium ratio. Further experiments will explore these effects more fully and, in particular, measure the temperature at which the fusion yield reaches a maximum. The objective of this project is to provide answers to recurring questions regarding the usefulness of muon-catalyzed fusion as a practical energy source.

17. GENERATION OF STIMULATED EMISSION IN THE SOFT X-RAY RANGE BY NONLINEAR PROCESSES WITH EXCIMER LASERS

UNIVERSITY OF ILLINOIS AT CHICAGO
Chicago, Illinois 60680

Charles K. Rhodes
Department of Physics

Date Started: September 15, 1983

Funding: FY '83 $413,000 for 2 years

Anticipated Duration: 2 years

High spectral brightness rare gas halogen (RGH) excimer lasers can be used to generate coherent extreme ultraviolet radiation by either harmonic generation mechanisms or direct multiphoton pumping of appropriate laser media. In order to demonstrate the basic characteristics of these two approaches, recent comparative measurements have been made. Extension of these results to both shorter wavelengths and higher power levels requires an extended study of the basic character of high order nonlinear processes in the ultraviolet. Recent studies of collision-free multiply-charged ion production with irradiation at 193 nm point to an anomalously strong energy coupling to high Z atoms with processes involving as many as 99 photons being observed. These findings strongly suggest that the direct excitation of inversions by appropriate multiquantum processes in the 40-80 eV range in certain atoms can be generated with existing laser instrumentation. This document proposes a two year experimental program to (1) determine the nature of the mechanisms leading to the anomalous ion production, (2) assess the limitations on the quantum state selectivity such processes can provide, and (3) attempt to observe genuine stimulated emission in the 40-80 eV range. Given the scaling characteristics of RGH media, success in this endeavor would imply the feasibility of a laboratory scale coherent source operating in the kilovolt range.

18. FREE ELECTRON LASER AT THE ETA*

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

A.M. Sessler and D. Prosnitz

Date Started: February 8, 1982

Funding: FY '83 $330,000 for 12 months

Anticipated Duration: 32 months

The purpose of this experiment is to develop a tapered-wiggler Free Electron Laser (FEL) as an efficient microwave source between 35 and 40 GHz. One important application of this source is in electron cyclotron resonance heating of thermonuclear plasmas. The Lawrence Livermore National Laboratory's Experimental Test Accelerator provides the high-current, high voltage (1 kA, 4 MeV) low emittance electron beam used to drive the FEL amplifier. The first year was devoted to building beam line components; the electron beam wiggler which is electromagnetic, has no iron, and is pulsed; and microwave input and output diagnostics. Initial operation was developed at 8 mm wavelength, with the capability of studying 2 mm and 4 mm in the future. Experimental runs with the apparatus were initiated in February 1983 and beam has been transported through the wiggler, oscillation (from noise) has been observed, and amplification (with a gain larger than unity) of an input microwave signal has been observed. Further experiments will be done to increase the gain of such a device, as well as to clarify the physics of an FEL amplifier.

*Experimental Test Accelerator at Lawrence Livermore National Laboratory.

19. AN APPROACH TO RECOVER STRATEGIC METALS FROM BRINE

LAWRENCE LIVERMORE NATIONAL LABORATORY
P.O. Box 808
Livermore, California 94550

Ellen Raber
Earth Sciences Department

Date Started: February 1, 1982

Funding: FY '83 $137,000 for 12 months

Anticipated Duration: 20 months

The objective of this project is to evaluate natural brines obtained from salt domes and geothermal sources as possible resources for some strategic metals. Based upon research efforts conducted last year, platinum was detected at near-commercial values of $\simeq$50 ppb in a brine from the Salton Sea Geothermal Resource, Imperial Valley, California. This brine is also rich in lithium, strontium and manganese. If possible, additional samples will be analyzed from other wells to determine the actual areal extent of platinum in the Salton Sea Geothermal Field. None of the other fluids (from 14 locations sampled elsewhere in the United States) contained interesting concentrations of strategic metals. Bench scale experiments are being conducted to determine the feasibility for recovery of the platinum by activated carbon, commerical reductive resins, iron reduction and electrolytic methods. Any viable method will need to be operational at 90^{o}C in the absence of oxygen. To date, Rohm and Haas Amborane-355 Resin has proven successful under these conditions. The cost-effectiveness of this and other methods will be evaluated. Additionally, a mini-field test is planned in conjunction with a developer to further evaluate the best extraction technique.

20. *DETECTION AND ENRICHMENT OF FRACTIONALLY CHARGED PARTICLES IN MATTER

LAWRENCE LIVERMORE NATIONAL LABORATORY
P.O. Box 808, L-482
Livermore, California 94550

Charles D. Hendricks
Y Division, Laser Program

Date Started: May 1, 1982

Funding: FY '82 $360,000 for 12 months

Anticipated Duration: 3 1/2 years

It is the objective of this experiment to search for fractional charges in matter and if they are found, to concentrate them for further experimental studies. Two vertical column vacuum systems are operational containing 3 meter and 5 meter long deflection plates. One system is reserved for use with very low vapor pressure liquid drops and the other is used with very low vapor pressure liquid drops and the other is used with higher vapor pressure liquids. Streams of equal mass drops have been passed vertically through the deflection system with transverse E fields of 25 kV/cm. Drop deflections have been observed which are consistent with integer electron charge differences between drops. Interactions between drops as a result of polarization by the transverse electric field have also been observed experimentally. To eliminate this source of irregularity in the drop deflections, the drop to drop spacing (which is normally about two drop diameters) is being increased to about 20 drop diameters by removing some of the drops from the stream. Because of the high rate of drop throughput (30 to 50 thousand drops per second) it is necessary to utilize electronic data acquisition. The computer-experiment interface is being designed and will be implemented.

*Projects 20 and 23 are cooperative interlaboratory projects.

21. PUMPING OF GAMMA-RAY LASERS: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS

LOS ALAMOS NATIONAL LABORATORY
Los Alamos, New Mexico 87545

G. C. Baldwin
Physics Division

Date Started: September 27, 1983

Funding: FY '83 $360,000 for 12 months

Anticipated Duration: 2 years

The power required to pump gamma-ray lasers could be significantly reduced, thereby enhancing the prospects for their early development, if a) a long-lived nuclear isomer, prepared in advance, could be rapidly converted to a short-lived state that emits recoilless gamma radiation; and/or b) internal conversion could be controlled. This research will investigate the preparation of nuclear isomers by selective laser photoionization, will study the possibility of their de-excitation by laser-induced Raman processes, and will attempt, by optical excitation of its electronic structure, to modify the internal conversion rate in the 73-eV isomer of ^{235}U.

22. LIQUID METAL THERMO-ACOUSTIC ENGINE

LOS ALAMOS NATIONAL LABORATORY
Los Alamos, New Mexico 87545

J. C. Wheatley
Physics Division

Date Started: September 27, 1983

Funding: FY '83 $240,000 for 12 months

Anticipated Duration: 3 years

This project is concerned with studying a new type of thermoacoustic heat engine using a liquid metal as the working substance. The thermophysical properties of liquid metals make them far superior to ideal gases as working substances in such an engine. Although the study is of fundamental interest it is also expected that this engine will be of technological importance, because it will produce electricity from heat with no moving parts and with an efficiency that is a substantial fraction of the Carnot efficiency. Currently efforts are under way to extend previous work on thermoacoustics in ideal gases to liquids, and efforts will soon begin on detailed computer design of an experimental engine with an electrical power output of about 1 kW.

23.*DETECTION AND ENRICHMENT OF FRACTIONALLY CHARGED PARTICLES IN MATTER

LOS ALAMOS NATIONAL LABORATORY
P.O. Box 1663
Los Alamos, New Mexico 87545

George Zweig
Theoretical Division

Date Started: May 1, 1982

Funding: FY '83 $100,000 for 12 months

Anticipated Duration: 3 1/2 years

The basic unit of electric charge is one third that of the electron. It is therefore natural to ask if isolated particles of fractional charges $\pm$ 1/3e, $\pm$ 2/3e, $\pm$ 4/3e. . . . exist freely as elements of the earth. William Fairbanks' group at Stanford University has concluded that they do. Negative fractionally charged particles are interesting because they could replace electrons in atoms, molecules and solids, leading to super-dense states of matter. Under certain circumstances they would even catalyze fusion reactions. This project is a combined theoretical and experimental effort to search for fractionally charged particles in a wide variety of materials, to determine which materials are most abundant in fractionally charged particles, and to enrich the fractional charge content of sample materials. The crystal chemistry of fractionally charged particles will be theoretically developed and those materials most likely to contain enhanced concentrations of fractionally charged atoms will be identified. These materials will then be obtained, analyzed and used as samples for the experimental studies.

*Projects 20 and 23 are cooperative interlaboratory projects.

24. MAGNETIC REFRIGERATION FOR EFFICIENT CRYOGEN LIQUEFACTION

LOS ALAMOS NATIONAL LABORATORY
P.O. Box 1663, MS M764
Los Alamos, New Mexico 87545

John A. Barclay
Group P-10

Date Started: February 1, 1982

Funding: FY '83 $340,000 for 12 months

Anticipated Duration: 3 1/2 years

The objective of this work is to consider conceptual designs, test models of those designs, and develop a data base for compact, reliable, high-efficiency magnetic refrigeration, with special emphasis on applying this technology to liquefaction of cryogens. Experiments are conducted to determine the magneto-caloric effect and the heat capacity of suitable solid magnetic working materials over the temperature range 1 to 300 K and at magnetic fields up to 9 T as well as the heat and fluid flow through beds of these materials. Three bed geometries are considered: porous beds made of small particles; many parallel sheets separated by small gaps; and a block with many circular channels. Additional efforts are directed toward: determination of parasitic heat losses; optimization of magnetic field configuration; design of heat exchangers, cryogenic pumps, and fluid entrainment suppressors; and development of new concepts (other than rotating and reciprocating devices) for magnetization/demagnetization. Samples of several gadolinium compounds with Curie temperatures from 300 to 4 K were fabricated. The density, Curie temperature, magnetization, magnetic susceptibility, heat capacity, and adiabatic magnetization/demagnetization temperature change for one of the samples, GdNi, have been measured. Similar measurements on the other samples are in progress.

25. ZONE-MELTING RECRYSTALLIZATION FOR SOLAR CELLS

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
77 Massachusetts Avenue
Cambridge, Massachusetts 02139

Henry I. Smith
Electrical Engineering & Computer Science

Date Started: September 1, 1982

Funding: FY '82 $200,000 for 24 months

Anticipated Duration: 2 years

The objective of this project is to develop a process for producing oriented silicon films suitable for low-cost solar cells. A new technique, zone-melting recrystallization, has been developed which produces crystalline silicon films having mobilities close to bulk values. Using a vertical-constriction technique, (100) texture has been obtained in films 60 μm thick. Single-grain films are produced by passing the molten zone through a lithographically-defined planar constriction. Lithographically-defined patterns have also been used to confine grain boundaries, dislocations and impurities to a set of narrow, parallel rejection channels spaced ~100 μm apart. An orientation-filtering technique has been developed to control azimuthal orientation. Electrical measurements have indicated that the films are free of deep-level-producing impurities and have acceptable minority carrier diffusion lengths. Our strategy is to produce high-quality crystalline silicon films on low-cost glass substrates. The glass substrate would serve as the cover of the final module.

26.*COGENERATION OF ELECTRIC ENERGY AND USEFUL CHEMICALS IN A FUEL CELL

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
77 Massachusctts Avenue
Cambridge, Massachusetts 02139

J. Wei
Department of Chemical Engineering

Date Started: September 1, 1980

Funding: FY '82 $100,000 for 12 months

Anticipated Duration: 4 1/3 years**

The conversion of the heat released by exothermic chemical reactions into electrical energy is becoming increasingly important in chemicals manufacture. Unfortunately, the conversion efficiency of traditional thermal cogeneration systems is thermodynamically limited and practical efficiencies may be quite small. Electrochemical cogeneration, in which a useful chemical product and electricity are produced simultaneously in a fuel cell, is not subject to this limitation. The present project investigates the concurrent electrochemical production of electricity with the oxidative dehydrogenation of ethylbenzene to styrene and butane to butadiene in zirconia fuel cells with appropriate catalytic electrodes.

*Project completed.

**Includes unfunded extension.

27. DEVELOPMENT OF DIRECT-CONTACT, HIGH EFFECTIVENESS DROPLET HEAT EXCHANGERS

MATHEMATICAL SCIENCES NORTHWEST, INC.
2755 Northup Way
Bellevue, Washington 98004

William J. Thayer III
Flow Technology Group

Date Started: July 1, 1981

Funding: FY '83 $257,000 for 12 months

Anticipated Duration: 3 years

A reliable technique for transferring heat between gas and liquid streams in the 1500-2000 K temperature range could greatly improve the efficiency of current power generation systems. Heat transfer between media in direct contact may eliminate many limitations of conventional heat exchangers which require intervening solid walls. The objective of this program is to characterize and evaluate techniques for providing high effectiveness heat transfer between high temperature droplets and counterflowing gas streams. A computer code has been developed for evaluating two-dimensional flow aspects of droplet and gas injection, column flow, and collection, convective and radiative heat transfer, and wall losses for direct-contact heat exchanger configurations. Tests have been conducted to characterize and evaluate processes which control the formation of uniform droplets of very viscous fluids which simulate molten refractories. Analysis and experiments are continuing to evaluate heat transfer and flow processes, materials issues, design constraints, and the economic impact of the direct-contact heat exchanger for several high temperature applications.

28. PERVAPORATION: A LOW-ENERGY ALTERNATIVE TO DISTILLATION

MEMBRANE TECHNOLOGY AND RESEARCH, INC.
719 Colorado Avenue
Palo Alto, California 94303

Richard Baker

Date Started: April 15, 1983

Funding: FY '83 $84,000 for 12 months

Anticipated Duration: 20 months

The object of this project is to develop selective pervaporation membranes. Pervaporation is a membrane separation process that could offer substantial energy savings compared to distillation. The principal problem inhibiting the development of pervaporation is the lack of suitably selective membranes. A series of provisional criteria for the selection of high-performance membranes has been developed. These criteria are being evaluated using model organic mixtures chosen to simplify the interpretation of the results. Thin film composite membranes made by the free-radical polymerization of single monomers will be used. Based on the experience obtained with these model mixtures we propose to determine the applicability of pervaporation to more economically significant organic mixtures. This data will be used to perform a technical and economic analysis of the process.

29. EXPERIMENTAL RESEARCH IN HIGH TEMPERATURE SOLAR THERMOCHEMICAL PROCESSING. HYDROGEN AND SULFUR FROM HYDROGEN SULFIDE

UNIVERSITY OF MINNESOTA
111 Church Street, S.E.
Minneapolis, Minnesota 55455

Edward A. Fletcher
Department of Mechanical Engineering

Date Started: July 16, 1982

Funding: FY '82 $229,000 for 24 months

Anticipated Duration: 2 years

Highly concentrated sunlight is uniquely suited for supplying process heat at very high temperatures. The efficiency with which process heat is used to effect endothermic processes increases as the temperature at which the heat is added increases. This project makes use of a highly-concentrating solar furnace to study the production of hydrogen and sulfur from hydrogen sulfide in a high-temperature effusional process. We have studied the effect of hydrogen sulfide and its decomposition and oxidation products, as well as admixed hydrocarbons, on material for reactor construction, constructed the major components of a reactor-separator and its appurtenances, and are evaluating various techniques for the construction of effusion membranes. We shall conduct experiments to test the efficacy of the process and evaluate the cost benefits which may be achievable by these kinds of processes vis-a-vis more conventional methods.

30. HOLOGRAPHIC TECHNOLOGY FOR SOLAR ENERGY CONCENTRATION

NATIONAL TECHNICAL SYSTEMS
12511 Beatrice Street
Los Angeles, California 90066

Tomasz Jannson
Research Division

Date Started: June 1, 1981

Funding: FY '83 $204,000 for 12 months

Anticipated Duration: 3 years

Research in this project is aimed at establishing the practical feasibility of using holographic technology (diffractive optics) for solar energy concentration. Very high reflection concentrators were fabricated in the first phase of the program and extinction rations of over 90% were achieved for on-axis holograms for the visible range. The objective during the second year is to build a bench scale photovoltaic solar energy conversion device using a holographic solar concentrator. Holographic solar concentrators with high concentration ratios will be fabricated with dichromated gelatin films. Measurements will be made on this system for system efficiency. Theoretical analysis is being conducted for nontracking type holoconcentrators and they will be fabricated in the third phase of this program.

31. HIGH-FLUX, EXTENDED-PULSE ION ACCELERATOR

UNIVERSITY OF NEW MEXICO
Albuquerque, New Mexico 87131

S. Humphries, Jr.
Department of Chemical and Nuclear Engineering

Date Started: September 27, 1983

Funding: FY '83 $267,000 for 3 years

Anticipated Duration: 3 years

A novel plasma source and ion injector gap geometry which may allow intense ion beam generation for pulselengths exceeding 1 ms will be studied. The pulselength is a factor of 1000 improvement over the present state-of-the-art. The source and injector utilize a radial magnetic field to confine a high density of trapped electrons. This allows transport of ion flux well above conventional space charge limits. The source operates as a cold-cathode discharge with good ionization probability because of the high electron density. A system to produce a 1 ms, 1 kA beam of He+ or heavier ions will be built. The 10 A/cm^2 beam will be extracted at 5 to 20 kV and a divergence less than 20 mrad.

32. MODIFICATION OF THE SURFACE TEMPERATURE BY AN ARTIFICIAL CIRRUS CLOUD

STATE UNIVERSITY OF NEW YORK
Albany, New York 12222

Bernard Vonnegut and Peter Chylek
Atmospheric Sciences Research Center

Date Started: September 1, 1980

Funding: FY '80 $244,000 for 36 months

Anticipated Duration: 3 1/3 years*

The objective of this project is to explore the practicality of using artificially formed cirrus clouds to achieve significant energy savings in densely populated areas. Meteorological data for about 10 years in the Albany area have been analyzed to determine how often the situation favorable for formation of an artificial cirrus cloud occurs. Preliminary results indicate that a suitable situation in the middle and upper troposphere occurs about 10 times per cold season. The combined effect of clearing clouds during the daytime and making cirrus clouds during nighttime gives a benefit-to-cost ratio of about 4/1 for the Albany area. For large metropolitan areas the benefit-to-cost ratio may be up to 40/1. Experimental work carried out at the University of Alaska's site at Fairbanks was concerned with observing the details of how light is scattered by clouds of water droplets and ice crystals. Analysis has also been carried out on about 10 years of data showing the effect of cirrus clouds over Mauna Loa on hourly average diffuse and direct solar radiation. This analysis can be used to suggest what effects artificial cirrus clouds would have on solar radiation reaching the surface. A radiative-convective climate model has been used to estimate the effect of increased cloudiness on the surface temperature, and radiative properties of ice clouds have been studied.

*Includes unfunded extension.

33. ENERGY SYSTEMS BASED ON POLYACETYLENE: RECHARGEABLE STORAGE BATTERIES AND SCHOTTKY BARRIER SOLAR CELLS

UNIVERSITY OF PENNSYLVANIA
3451 Walnut Street
Philadelphia, Pennsylvania 19104

A. G. MacDiarmid
Department of Chemistry

Date Started: March 1, 1981

Funding: FY '82 $101,000

Anticipated Duration: 3 years

The objective of this project is to investigate the chemical, electrochemical, electrical and optical properties of the novel conducting polymer $(CH)_x$, polyacetylene, with a view toward applications in two areas: rechargeable storage batteries made with $(CH)_x$ electrodes, and Schottky barrier solar cells made with $(CH)_x$. Work during FY 1983 continued to focus on the rapid progress in the area of $(CH)_x$ batteries. Coulombic efficiency, constant current discharge characteristics, energy density, maximum power density and the relationship of cell potential to degree of reduction of a partly reduced polyacetylene, $[Li_y(CH]_x (y \leq 0.1)$ cathode in a cell of the type $[Li_y(CH)_x/LiClO_4/Li$ were determined. The $[Li_y(CH)]_x$ $(y \leq 0.1)$ electrode appears to be stable indefinitely in an electrolyte of 1M $LiClO_4$ in tetrahydrofuran in a sealed cell. The stability and reversibility of the reduced polyacetylene electrode holds promise for its use as an anode active material. Current investigations include the construction of rechargeable battery cells using $[Li_y(CH)]_x$ or $[Na_y(CH)]_x$ anodes together with titanium disulfide (TiS_2) cathodes.

34. IMPLODING PLASMA X-RAY LASER

PHYSICS INTERNATIONAL
2700 Merced Street
San Leandro, CA 94577

Raymond Dukart

Date Started: September 1, 1981

Funding: FY '83 $375,000 for 12 months

Anticipated Duration: 2 1/2 years

A collisionally pumped Ne-like krypton x-ray laser scheme is being investigated using an imploded plasma source (~4 cm x 0.5 mm). The implosion is driven by the 5 TW Defense Nuclear Agency PITHON electrical pulse generator. According to theories developed at Lawrence Livermore National Laboratory, the measured plasma temperature ($T_e \sim 1$ keV) and density ($N_e \sim 10^{21}$ electrons/cm^3) are nearly ideal for producing population inversions in XUV (~83-100 eV) 3-3 Ne-like krypton transitions. Analysis of the time integrated XUV spectra show the presence of Al-like through O-like krypton states. Time-resolved XUV spectra have been obtained, completing identification of the 3-3 Ne-like spectra and provide data on the Ne-like krypton line widths for input into the theoretical laser model. Work is also continuing on further improving the plasma implosion simultaneity and instantaneous high temperature plasma length (>2.4 cm during a 2 ns frame has previously been obtained).

35. SOFT X-RAY LASING ACTION IN A CONFINED PLASMA COLUMN

PRINCETON UNIVERSITY
Princeton, New Jersey 08544

Szymon Suckewer
Plasma Physics Laboratory

Date Started: September 13, 1979

Funding: FY '83 $305,000 for 12 months

Anticipated Duration: 4 years

The objective of this project is an experimental investigation of lasing action in the soft x-ray spectrum region at wavelengths 182 A, 135 A and 520 A corresponding to the 3→2, 4→2, and 4→3 transitions in the CVI ion. The basic idea is to use a multi-Z (e.g., carbon, oxygen) thin plasma column confined by a strong longitudinal magnetic field (100 kG), first heated by a CO_2 laser and then cooled rapidly by radiation losses. Calculations indicate a total gain in excess of 100 for the 3→2 transition, in excess of 10 for the 4→2 transition, and in excess of 300 for the 4→3 transition for a 10 cm long plasma column heated by a 10-20 GW CO_2 laser beam. Experiments showed good plasma confinement in magnetic fields 50-100 kG and effective radiation cooling of such a plasma, especially with additional small amounts of higher-Z elements such as Ar or Xe. Measurements of gain for CVI 4 3 (520 A) and 3→2 (182 A) transitions indicate the possibility of obtaining a high gain for 4 3 transitions, and also for the 3→2 transitions with improved CO_2 laser optics.

36. DEPOSITION OF HIGH QUALITY $CuInSe_2$ BY SPRAY PYROLYSIS

RADIATION MONITORING DEVICES, INC.
44 Hunt Street
Watertown, Massachusetts 02172

Gerald Entine

Date Started: September 15, 1982

Funding: FY '83 $116,000 for 12 months

Anticipated Duration: 2 years

The ultimate success of any terrestrial photovoltaic energy conversion approach requires that the following factors be satisfied: 1) high individual solar cell conversion efficiency, 2) low cost per unit area to produce the cells, 3) adequate availability of the constituent materials to produce the cells, 4) long term stability. This project is a proof-of-concept effort to show that spray pyrolyzed $CuInSe_2$ can meet all of the requirements. $CuInSe_2$ is a promising solar cell material and spray pyrolysis is a technique well-suited for use in a manufacturing process.

37. IONIZATION FRONT ACCELERATOR

SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Craig L. Olson
Plasma Theory Division - 1241

Date Started: June 1, 1981

Funding: FY '83 $110,000 for 6 months

Anticipated Duration: 3 years

The objective of this project is to accelerate ions to high energies using the large space charge field (~100 MV/m) from the potential well at the head of an intense relativistic electron beam (IREB). The Ionization Front Accelerator (IFA) accomplishes this by using laser photoionization of a special working gas to control the motion of the potential well. A second generation system (IFA-2) is being brought into operation. This system includes an IREB machine (1.0 MV, 30 kA, 30 nsec) with laser-triggered switches, and a beam conditioning cell to steepen the current rise time; an experimental cell with Cs as the working gas; and a dye laser (852.1 nm) to pre-excite the Cs, an XeCl laser (308 nm) to photoionize the excited Cs, and a Pockels deflector to provide a continuous sweep for the XeCl laser beam. The IREB is operational with a command firing jitter of 1 nsec and a conditioning cell current rise time of < 3 nsec. The experimental cell and Cs ovens are complete, the dye laser and XeCl laser are operational, and testing of a high voltage driver for the deflector is in progress. After system check out, IFA-2 experiments with a 30 cm sweep length will commence, complete with ion diagnostics.

38.*RELIABLE, LOW-COST, LOW POWER CRYOCOOLER TO REACH 4.0 KELVIN

S.H.E. CORPORATION
4174 Sorrento Valley Blvd.
San Diego, California 92121

Ronald E. Sager

Date Started: September 30, 1980

Funding: FY '82 $121,000

Anticipated Duration: 2 1/2 years

The goal of this project is to develop a cryocooler suitable for operating superconducting instrumentation below 5 Kelvin without the requirement for liquid helium cooling. Potential applications include geophysical prospecting using magnetotelluric measurements, magnetic borehole mapping, and interborehole electromagnetic propagation measurements. In the past year the physics of nonmagnetic cryocoolers was investigated, starting from room temperature, and a cooler is now operating at 7 Kelvin. Experiments are underway on innovations which should substantially improve the low temperature performance of the cryocooler and permit mounting a superconducting magnetic sensor on the cryocooler for demonstration purposes. Work has also started on the design of an experimental model cooler which is expected to evolve eventually into a very reliable instrument capable of operating continuously for years without maintenance or failure.

*Project completed.

39. PLANAR FLOW CASTING OF SHEET SILICON FOR PHOTOVOLTAIC CELLS

SOURCE TECHNOLOGY APPLIED METALLURGICALS, INC.
SOLAMAT DIVISION
885 Waterman Avenue
East Providence, Rhode Island 02914

Mandayam C. Narasimhan

Date Started: August 1, 1982

Funding: FY '83 $208,000 for 12 months

Anticipated Duration: 2 years

The object of this research program is to evaluate the castability of silicon sheets for photovoltaic application by the planar flow casting process and a newly developed roller quench casting process. The planar flow casting process was found to be inoperative in ambient. This is due to the oxidation of the surface of the melt which results in poor thermal contact between the chill wheel and the silicon melt. Ribbons produced in inert atmosphere by this process show columnar grain structure with the grain dimensions in the range of 1 - 10 microns. The newly developed roller quench casting process casts wide polycrystalline silicon sheets (approximately 2" in width) with thicknesses of 15 - 25 mils at casting speeds of 50 - 100 feet per minute. The initial results of the sheet characterization show that the grain structure in these sheets in columnar, the grain dimensions are in the millimeter range, the sheets are p-type and their electrical resistivity is in the range of 0.1 - 10 ohm-cm. The resistivity of these sheets is maintained within the same order of magnitude as that of the starting material. Solar cells are being fabricated and characterized to assess the photovoltaic quality of these silicon sheets.

40. SYNTHESIS AND PHOTOELECTROCHEMICAL CHARACTERIZATION OF SEMICONDUCTING GROUP VIII TRANSITION METAL CHALCOGENIDES AND PNICTIDES

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

Bruce Parkinson
Photoconversion Research Branch

Date Started: September 26, 1983

Funding: FY '83 $143,000 for 12 months

Anticipated Duration: 2 years

Semiconducting electrodes, which are illuminated in an electrolyte solution, are capable of harvesting solar energy and converting it directly to electrical power or storable chemical fuels. Previous efforts in this area have concentrated on semiconducting materials which have been available because of their use in solid state devices, but these materials are not necessarily the best materials for photoelectrochemical applications. We are synthesizing and characterizing new semiconducting materials specifically for photoelectrochemical applications. The semiconductors are made from a Group VIII metal (Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt), combined with a chalcogen (S, Se, Te) or a pnicogen (P, As). The metals are chosen because they have catalytic activity for many of the important photoelectrosynthetic reactions, such as water photolysis and carbon dioxide reduction. The pnictides and chalcogenides of these metals should have favorable bandgaps and have stability against photocorrosion.

41. MULTIFUNCTION WALL SYSTEM FOR APPLICATION WITH SOLAR HEATING AND GROUND COOLING

VIRGINIA POLYTECHNIC INSTITUTE
AND STATE UNIVERSITY
Blacksburg, Virginia 24061

James F. Riley and Gary E. Day
College of Architecture and Urban Studies

Date Started: September 1, 1981

Funding: FY '81 $105,000 for 18 months

Anticipated Duration: 3 1/4 years*

The purpose of this project is to establish the scientific feasibility of the concept of a multifunction wall system (for application with solar heating and ground cooling) as applied to contemporary design and construction methods. The concept of the system is to expand the use of structure and enclosure elements of a building to function additionally as: the ductwork for the solar heated or earth cooled air, the heat transfer membrane between the heated or cooled air and the living environment of the building, the heat storage medium (in winter), and the temperature leveling and control medium. During FY '83 activity has focused on monitoring and evaluating a small test building at Virginia Tech. The data derived from this testing is being used to generate system performance models relative to the heating and cooling functions.

*Includes unfunded extension.

42. A METHOD OF ACHIEVING SUPER-PRESSURES BY ADVANCED GASDYNAMIC TECHNIQUES

UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

A. Hertzberg, A.P. Bruckner and Y.K. Rao
Aerospace and Energetics Research Program

Date Started: September 27, 1982

Funding: FY '83 $131,000 for 12 months

Anticipated Duration: 1 1/2 years

A new gasdynamic concept for the generation of isentropic pressure pulses in the range of tens of kilobars to several megabars, with durations of the order of microseconds, will be investigated. The technique involves the generation of an isentropic wave system at relatively low pressures (i.e., less than 5-10 kbar) in a medium of low acoustic impedance (e.g., gaseous hydrogen) and the propagation of this wave system through media of increasing impedance, thereby generating very high pressures in the final, maximum impedance medium. The succession of media may include gases, liquids and solids. This method could be used to measure equation of state data along isentropes at very high pressures. The technique also has the potential for creating heretofore inaccessible states of matter which may have important industrial or energy applications, as well as for applications in controlled thermonuclear fusion.

43.*ANALYSIS OF IMPACT FUSION TARGET DYNAMICS

UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

F.L. Ribe
Aerospace and Energetics Research Program

Date Started: April 15, 1983

Funding: FY '83 $84,000 for 12 months

Anticipated Duration: 3 years

In conjunction with rail-gun experiments on macroparticle acceleration we study the conversion of rectilinear projectile motion to a spherical or quasi-spherical implosion. Initial work involves one-dimensional numerical solutions of the hydrodynamic and transport equations, matched at the interface of a compressible metallic shell and an internal fusile gas for planar and spherical geometry. Later work will involve the two-dimensional problem of rectilinear and quasi-spherical motion.

*Projects 43 and 44 are cooperative interlaboratory projects.

44.*INVESTIGATION OF HIGH-VELOCITY ELECTROMAGNETIC LAUNCHER BEHAVIOR FOR USE IN IMPACT FUSION

WESTINGHOUSE R & D CENTER
1310 Beulah Road
Pittsburgh, Pennsylvania 15235

Ian R. McNab
Electrotechnology Department

Date Started: July 18, 1983

Funding: FY '83 $394,000 for 12 months

Anticipated Duration: 4 years

It has been proposed that thermonuclear fusion can be ignited by impact of a deuterium-tritium pellet by a one-half gram heavy-metal projectile at velocity of about 200 km/s. The objective of this program is to investigate the scientific and technological problems associated with the electromagnetic acceleration of a 1 g projectile to 30 km/s using a multi-stage railgun, and to obtain scaling relationships for attaining higher velocity. A companion program to explore theoretically impact physics at high velocities and target design concepts to achieve thermonuclear burn is undertaken at the University of Washington. The velocity of 30 km/s is considered to be the minimum velocity at which impact will yield detectable quantity of neutrons.

*Projects 43 and 44 are cooperative interlaboratory projects.

OFFICE OF BASIC ENERGY SCIENCES

DIVISION OF ADVANCED ENERGY PROJECTS

Fiscal Year 1983 Program Data

FY '83 Budget

Operating Funds.....$8,310,000

Capital Equipment Funds.....$ 300,000

Distribution of Projects by Institutional Sector

Universities	37%
Small Business	26
Other Industry	9
DOE Laboratories	28
	100%

INSTITUTIONAL INDEX
(Project Numbers)

Bend Research, Inc	1,2
Brookhaven National Laboratory	3,4,5
California, University of (Irvine)	6
California Institute of Technology	7
Case Western University	8
Cornell University	9
Dynatech R/D Company	10
EIC Laboratories, Inc.	11
Energy & Environmental Engineering, Inc.	12
General Atomic Company	13
George Washington University	14
GT-Devices	15
Idaho National Engineering Laboratory	16
Illinois, University of (Chicago)	17
Lawrence Berkeley Laboratory	18
Lawrence Livermore National Laboratory	19,20
Los Alamos National Scientific Laboratory	21,22,23,24
Massachusetts Institute of Technology	25,26
Mathematical Sciences Northwest, Inc.	27
Membrane Technology and Research, Inc.	28
Minnesota, University of	29
National Technical Systems	30
New Mexico, University of	31
New York State, University of (Albany)	32
Pennsylvania, University of	33
Physics International	34
Princeton University	35
Radiation Monitoring Devices, Inc.	36
Sandia National Laboratories, Albuquerque	37
S.H.E. Corporation	38
Source Technology Applied Metallurgicals, Inc. Solamat Division	39
Solar Energy Research Institute	40
Virginia Polytechnic Institute and State University	41
Washington, University of	42,43
Westinghouse R & D Center	44

K. Biological Energy Research (BER) Subprogram

1. **What is the detailed budget structure of the BER subprogram? What types of work are funded by each of these budget categories?**

   Answer: The BER budget is broken down into two categories - operating and capital equipment. The size of the program is such that subcategories are appropriate considering the fact that the work is closely interlocked. The objectives of the Biological Energy Research subprogram are a) to develop an understanding of fundamental biological phenomena in plants and microorganisms that will underpin the development of improved strategies for enhanced productivity of renewable resources; b) to generate a base of fundamental information on which to construct new and improved microbiological conversions of materials into useful fuels and chemicals; and c) to explore and understand basic biological phenomena which may be employed in developing biosystems as substitutes for energy intensive chemical processes.

2. **For the period FY 1981 - FY 1985, please provide operating expenses, capital equipment, and construction funding for each budget category identified in question 1.**

   Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
BIOLOGICAL ENERGY RESEARCH					
OPERATING EXPENSES	$ 7237	$ 8420	$ 9500	$ 10580	$ 12490
CAPITAL EQUIPMENT	400	410	370	400	560
SUBPROGRAM TOTAL	7637	8830	9870	10980	13050

3. **For the period FY 1981 - FY 1985, please identify, by budget category and by facility, that portion of BER funding that goes for the support of facilities, such as the National Synchrotron Light Source, etc.**

   Answer: In the period FY 1981 - FY 1985 none of the BER subprogram funding has been used for support of facilities.

4. **For the period FY 1981 - FY 1985, please provide, by budget category and by DOE laboratory, the amount of BER funding going to DOE laboratories.**

   Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
BIOLOGICAL ENERGY RESEARCH
LABORATORIES
(B/A In thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC06 BIOLOGICAL ENERGY RESEARCH					
OPERATING EXPENSES					
BROOKHAVEN NATIONAL LAB	$ 830	$ 850	$ 915	$ 980	$ 1200
LAWRENCE BERKELEY LAB	790	840	910	1011	1200
LAWRENCE LIVERMORE NAT LAB	0	0	20	0	0
LOS ALAMOS NATIONAL LAB	0	0	0	0	200
OAK RIDGE NATIONAL LAB	0	150	200	200	200
SERI	100	100	105	105	120
35KC06 BIOLOGICAL ENERGY RESEARCH					
CAPITAL EQUIPMENT					
BROOKHAVEN NATIONAL LAB	25	25	70	50	50
LAWRENCE BERKELEY LAB	50	60	50	50	50

5. **For the period FY 1981 - FY 1985, please provide, by budget category and by company, the amount of BER funding going to industry.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
BIOLOGICAL ENERGY RESEARCH
INDUSTRY
(B/A In thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
KC06 BIOLOGICAL ENERGY RESEARCH					
OPERATING EXPENSES					
BATTELLE COLUMBUS LAB	$ 0	$ 98	$ 0	$ 0	$ 0
MARTIN MARIETTA CORP	80	91	86	95	0

6. **For the period FY 1981 - FY 1985, please provide, by budget category and by institution, the amount of BER funding going to universities.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
BIOLOGICAL ENERGY RESEARCH
UNIVERSITIES
(B/A In thousands)

BIOLOGICAL ENERGY RESEARCH

KC0600

OPERATING EXPENSES

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
BRANDEIS UNIV	$ 41	$ 42	$ 49	$ 53	$ 57
CALIF UNIV OF BERKELEY	0	0	82	85	0
CALIF UNIV OF DAVIS	40	20	60	60	0
CALIF UNIV OF IRVINE	135	125	134	142	0
CALIF UNIV OF LOS ANGELES	134	145	168	87	87
CALIF UNIV OF RIVERSIDE	5	0	3	4	0
CALIF UNIV OF SAN DIEGO	125	125	50	0	0
CALIF UNIV OF SANTA CRUZ	46	0	0	0	0
COLORADO UNIV OF	245	270	300	351	0
CORNELL UNIV	199	213	199	163	66
FLORIDA STATE UNIV	74	116	75	0	0
FLORIDA UNIV OF	60	58	69	0	0
GEORGIA UNIV OF	434	474	603	571	414
HARVARD UNIV	55	128	120	73	0
IDAHO UNIV OF	48	58	88	73	75
ILLINOIS UNIV OF	430	495	450	471	196
INSTITUTE OF PAPER CHEM	0	44	31	0	0
IOWA STATE UNIV - AMES	0	61	54	0	0
KENTUCKY UNIV OF	0	0	28	0	71
LEHIGH UNIV	0	0	69	83	0
MARINE BIOLOGICAL LAB	0	0	20	0	0
MARQUETTE UNIV	22	16	0	0	0
MARYLAND UNIV OF	0	58	63	64	0
MASSACHUSETTS UNIV OF	75	75	77	0	0
MICHIGAN STATE UNIV	1450	1600	1730	1750	1900
MINNESOTA UNIV OF	118	158	279	178	74
MISSOURI UNIV OF	56	55	72	67	68
MT SINAI SCH OF MEDICINE	69	0	78	73	77
NEBRASKA UNIV OF	50	101	116	105	0
NEW YORK ST UNIV OF BROOKLYN	81	85	90	0	0
NORTH CAROLINA STATE U	36	0	0	0	0
NORTH CAROLINA UNIV OF	83	80	85	87	0
NORTHWESTERN UNIV	0	0	0	60	0
OHIO STATE UNIV	64	63	63	0	0
OKLAHOMA UNIV OF	50	0	36	47	0
PENNSYLVANIA STATE UNIV	0	0	0	62	0
PENNSYLVANIA UNIV OF	79	80	80	82	83
PUERTO RICO UNIV OF	35	0	0	0	0
PURDUE UNIV	80	34	200	160	80
ROCKEFELLER UNIV	75	79	85	100	0
RUTGERS UNIV	75	120	52	55	0

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
SOUTHERN ILL UNIVERSITY	0	62	60	62	0
STANFORD LELAND JR UNVR	66	166	143	79	0
TENNESSEE UNIV OF	- 6	0	0	0	0
UTAH STATE UNIV	75	67	81	70	0
WASHINGTON STATE UNIV	0	111	112	72	0
WASHINGTON UNIV OF	216	145	205	207	0
WASHINGTON UNIV ST LOUIS	139	129	133	65	0
WISCONSIN UNIV OF	236	277	385	320	212
35KC06 BIOLOGICAL ENERGY RESEARCH					
CAPITAL EQUIPMENT					
COLORADO UNIV OF	150	150	100	0	0
MICHIGAN STATE UNIV	175	175	150	250	200

7. **For the period FY 1981 - FY 1985, please provide, by budget category and by agency, the amount of BER funding going to other agencies.**

Answer: Please see the table below for the requested information.

BASIC ENERGY SCIENCES
BIULOGICAL ENERGY RESEARCH
FEDERAL
(B/A in thousands)

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
BIOLOGICAL ENERGY RESEARCH					
KC0600					
OPERATING EXPENSES					
AGRICULTURE US DEPT OF	$ 0	$ 0	$ 41	$ 43	$ 0
NAT INST OF GEN MED SCI	0	40	40	40	0

8. **How does the research funded by the Biological Energy Research subprogram differ, complement, supplement, or overlap biological research funded by the Solar Energy or other DOE programs, or by other agencies such as the National Science Foundation and the USDA?**

Answer: The BER program supports research in the plant sciences and microbiology designed to generate the data base for improved and new biosystems relating to energy conversion and conservation.

The BER program has a number of areas of particular concentration that distinguishes it from other programs in government. These include basic mechanisms of methanogenesis, genetics of anaerobes involved in fermentations, plant stomatal physiology, plant cell wall studies and, in addition, it supports the unique premier integrated plant science laboratory in the country at Michigan State University (cited in OTA report "Commercial Biotechnology: An International Analysis", page 349, 1984).

While a number of the BER identified areas are covered to some degree by NSF and USDA, the work is complementary. Continuing interchanges (monthly meetings and regular telephone contacts) among the three agencies has assured that unnecessary overlap does not occur. Likewise, within DOE, there are contacts maintained with the Biomsss Energy Technology Division and the Office of Health and Environmental Research to insure prudent use of funds and avoidance of duplication.

9. **What types of formal and informal advisory groups are employed to assure that the subprogram is of high quality and coordinated with the research carried out at other agencies and within other parts of DOE? If any formal advisory groups exist, please provide a listing of the current membership.**

Answer: The Biological Energy Research (BER) Division uses numerous reviewers to assess the scientific quality of proposals and ongoing projects. In FY 1983 over 550 researchers in the country and abroad were used for review purposes either by mail, workshops, or as site visit reviewers. In addition, the program holds a workshop triennially to overview the entire program quality and discuss possible directions for the program. The individuals serving on these workshops are highly respected members of the research community from universities and industry. None are contractors or grantees.

A regular monthly meeting is held for individuals from different agencies involved in the support of plant science. At these meetings, each agency has the opportunity to present the scope of their programs, plans for the future and other information. These associations have created an atmosphere for easy exchange and coordination. The director of the BER program also serves on the steering committee of the USDA Competitive Grants Program and has also appeared before the USDA Users Advisory Board and the NAS Board on Agriculture. In summary, the information exchange is excellent about the BER program and those related programs in other agencies. There is also easy exchange of information within DOE among BER, the Office of Health and Environmental Research, and Biomass Energy Technology.

10. **What has DOE done towards planning an enhanced BER program?**

Answer: BER program growth has been steady and moderate. With the abundance of unsolicited proposals received, it has been possible to build the program with only excellent projects as determined by peer review. The BER plans for the future are best outlined in a paper published in Biomass 1 17 (1981), co-authored by the BER director. In addition, the triennial workshop and developments in technical areas provide "course correcting" influences.

11. **What funding levels would be required to conduct such an enhanced BER program?**

Answer: Since we do not know what budget packages will go forward for FY 1986 and future years, no budget estimates can be reasonably provided.

12. **Please provide a copy of the latest BER research summaries.**

Answer: Enclosed is the requested information.

Annual Report and Summaries of FY 1983 Activities Supported by the Division of Biological Energy Research

October 1983

INTRODUCTION

The mission of the Biological Energy Research (BER) program is to provide support for fundamental studies in biology oriented towards energy conversion and conservation to underpin future developments in energy related biotechnology. The BER program aims at comprehending biological principles and mechanisms rather than the development of specific technological processes. Implicit in the program is the need for a reciprocal flow of information between BER and those in the technologies about new findings, research needs and trends to avoid isolated paths of endeavor. This is accomplished by emphasizing openness and promptness of reporting research results, participation in interactive meetings and encouragement of investigators to exchange ideas broadly with others and particularly with researchers in industry.

At approximately three year intervals BER sponsors a workshop on research directions to examine the current status of the program, the relationship of recent advances in research to the BER program and what promising new directions are appropriate. In December 1982 the BER program sponsored such a workshop at the Smithsonian Institution's Belmont Conference Center near Baltimore, Maryland. The participants were from academia and industry and represented a number of disciplines. No BER contractors were involved. A number of research areas were pinpointed for attention, including many of those presented in the last year's (Fiscal Year 1982) annual report DOE/ER-0147:

> "Some examples of the research priority areas identified include: 1) definition of stress effects in plants at the biochemical and biophysical levels, and including adaptive mechanisms, 2) the biosynthesis and biodegradation mechanisms of the key natural polymers, cellulose, lignin and other polysaccharides, 3) the development of better understanding of the genetics of those microbes responsible for degradations and fermentations, especially anaerobic microorganisms, 4) the physiological genetics and biochemistry of important processes in both plants and microbial species, and 5) interactive relationships between different species of organisms as with plant host-pathogens, microbial consortia, and plant-soil microbes with emphasis on recognition events, and reciprocal flows of information and substrates. In addition to these areas the BER program maintains a significant stake in photosynthesis (the driving force of biological processes), and other energetics research, plant growth and development mechanisms, genetics of plant systems, microbiological studies on metabolic regulation, thermophily and other areas as will be seen in the following pages of the report."

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Also included were a number of research topics to be found in a recent National Academy of Sciences COSEPUP (Committee on Science, Engineering and Public Policy) report. A number of other points were brought out in the BER workshop. There was considerable concern expressed about the need for more collaboration between investigators in the plant and microbiological sciences and those in other disciplines. The rationale for this suggestion is the perceived growing complexity of research problems that necessitate broader thinking and input for more substantial progress. Of particular note was the view that plant scientists, in general, were not availing themselves of state-of-the-art instrumentation and techniques. In some cases they may be unaware of the kinds of instrumentation and capabilities that are available.

Acting on a suggestion of the Belmont meeting participants, a follow-on workshop on Plant Science and Instrumentation was convened at the National Synchrotron Light Source at Brookhaven National Laboratory (BNL) on 14-15 July 1983. The BNL workshop brought a group of plant scientists together with a group of workers deeply involved with instrumentation development and application. The interaction included plant scientists discussing the types of measurements that would be valuable in physiological and biochemical research if suitable techniques and instrumentation were available. The instrumentation oriented researchers discussed the versatility, potentialities and attributes of a number of representative techniques. Out of this meeting emerged several collaborative ideas. The summary report of this workshop, which is expected to be completed in fall 1983, will also contain several suggestions about how the generic issue of plant science and instrumentation might be attacked.

As mentioned above, during the Fiscal Year 1983 additional recognition of the importance of plant science research and the opportunities available was documented in a report under the auspices of the Office of Science and Technology Policy and the National Science Foundation through the National Academy of Sciences COSEPUP. That report confirmed the premises upon which the BER program and certain other research efforts sponsored by NSF and USDA are based. The research agenda identified is broad in scope. The fundamental research issues are relevant not only to agricultural interests but also to research programs in which the long term objectives relate to renewable resources (biomass) destined for use as fuels and chemicals. One inevitable question is how to coordinate work of several agencies that seems to be similar. In this case the question has been resolved. Since 1978 there has been in existence an Interagency Plant Science Committee which was organized not by mandate but by the initiative of individuals from several agencies who recognized the neglected state of plant science research and foresaw the major practical opportunities that would evolve from the support of fundamental plant science research. This interagency group meets monthly

to discuss numerous aspects of plant science research including research areas, manpower, facilities, equipment and a broad array of other topics. There is prompt and free exchange of information about various agency policies and funding so that each agency is apprised of what other agencies are doing. Clearly the mechanism for coordination exists and is operative.

Some representative contributions of BER contractors during the FY 83 period include the following: a) Progress was made in modifying the Agrobacterium tumefaciens Ti plasmid as a vector in the transfer of DNA in higher plants. The plasmid was "disarmed" by genetically altering that information which is responsible for unwanted tumor formation in recipient plants. In addition it was demonstrated that antibiotic resistance as a representative genetic character may be transferred by the Ti plasmid to a recipient plant culture (see project #72). b) By using appropriately constituted genetic lines of maize it has been possible by following male sterility restorer function to measure for the first time the frequency and character of genetic transposition events in a higher organism (see project #35). c) The gene coding for susceptibility to the herbicide atrazine in higher plants has been identified, cloned and sequenced. A mutant gene which is responsible for resistance to the herbicide has likewise been studied. The difference between the two is one nucleotide in the DNA sequence (see projects #99 and #105). d) Amino acid sequences of a number of proteins of the smallest functional photosynthetic particle, known as the reaction center, of the photosynthetic bacterium Rhodopseudomonas capsulata have been determined by cloning and sequencing the corresponding DNA. This information has led to new insights concerning the structural and functional nature of the proteins in photosynthesis (projects #95 and #98).

A number of other activities which are not listed in the summaries were funded during FY 83. These include:

1) Cold Spring Harbor Laboratory, partial support of a workshop entitled "The Genetics and Molecular Biology of Chlamydomonas" which was held June 26-30, 1983.

2) University of California, Riverside, partial funding for 6th Annual Symposium in Botany and Plant Sciences "Biosynthesis and Function of Plant Lipids", held January 13-15, 1983.

3) University of Minnesota, partial support for the "Fourth International Symposium on Microbial Growth on One-Carbon Compounds" held September 6-10, 1983.

4) Marine Biological Laboratory, partial funding for "A Microbial Ecology Summer Research Program with Special Emphasis on Studies with Anaerobic Microorganisms" held June 19 - August 26, 1983, Woods Hole, Massachusetts.

5) National Academy of Sciences, partial support of "Convocation on Genetic Engineering of Plants: Agricultural Research Opportunities", held at the National Academy of Sciences, May 23-24, 1983.

In the course of FY 83 a total of 71 new research proposals were received and 12 funded. While the BER program continues to grow modestly it is also subject to many of the constraints faced by other programs in active areas.

	No. of Projects	FY 83 Funding (in thousands of $)	% of Total Funds
University Contracts	73	5147	54
Michigan State University Plant Research Laboratory	11	1675	18
National Laboratories Brookhaven National Lab Lawrence Berkeley Lab Oak Ridge National Lab	15	2045	22
Solar Energy Research Inst.	1	105	1
Other Research Institutions (federal, state, industrial, non-profit)	10	422	4
Conferences and miscellaneous	6	106	1
TOTAL	116	9500	

A few words need to be said concerning the manner in which projects are listed as summaries. All projects which were active in Fiscal Year 1983 are listed including several which were funded with FY 82 monies. The funding levels indicate total costs. With respect to projects which are carried on in facilities such as Brookhaven National Laboratory,

Oak Ridge National Laboratory, and the Lawrence Berkeley Laboratory the funding levels will appear deceptively high compared to university projects inasmuch as oftentimes salaries of the principal investigators are included in the total funding figures. If there are any questions about the technical aspects of any of the projects listed these may be pursued by contacting the principal investigator.

There is an obligation, a most pleasant one, to express once again our deep appreciation to the large number of scientists both in the United States and abroad who have provided assistance to the BER program during the past year. Without the help in reviewing the technical quality of proposals, both newly submitted and on-going ones, it would be virtually impossible to achieve the high quality program that exists.

Questions about the overall Biological Energy Research program should be directed to:

Dr. Robert Rabson
Division of Biological Energy Research
Office of Basic Energy Sciences, ER-17, GTN
U. S. Department of Energy
Washington, D. C. 20545
Phone: (301)353-2873

1

1. U. S. DEPARTMENT OF AGRICULTURE
Ithaca, New York 14853

REGULATION OF EXPRESSION OF A SOYBEAN STORAGE PROTEIN SUBUNIT GENE. — $40,637
John F. Thompson and James T. Madison
Plant, Soil and Nutrition Laboratory

The objective of this research is to understand the regulation of a plant gene. In cotyledon culture, the 8-subunit of the 7S storage protein of soybeans is normally present. Addition of methionine to the basal medium results in the absence of the 8-subunit. Cotyledons will be cultured on basal medium with and without methionine and will be switched from medium without methionine to medium with methionine and vice versa to obtain evidence as to whether the effect is due to transcription, translation, or post translational effects. Messenger RNA from cotyledons grown without and with methionine will be tested for the presence of mRNA for the 8-subunit (by in vitro wheat germ system) and for 8-mRNA precursors (by hybridization to a cDNA clone). The possibility that post-translational processes are inhibited by methionine will be determined by use of 8-subunit specific antibodies.

2. BATTELLE COLUMBUS LABORATORIES
Columbus, Ohio 43201

COMPLEXES OF CHLOROPHYLL DERIVATIVES WITH HEME APOPROTEINS — $98,000 (FY 82 funds)
Robert H. Pearlstein
Organic and Polymer Chemistry Section

The chlorophyll (Chl) in either an antenna or a reaction center (RC) protein complex displays a red-shift of the longest-wavelength peak in its absorption spectrum (relative to the corresponding monomeric Chl in a solvent) that is difficult to explain in terms of Chl-Chl interactions. Because these anomalous redshifts are probably caused by a mechanism that, in RC complexes, helps to stabilize primary electron transfer, we are investigating the possibility that the redshift results from specific Chl-protein interactions, and exploring any connection between such interactions and the redox properties of primary donor Chl. Initial work with complexes of Chl derivatives and heme apoproteins led to the development of several models for Chl-protein interactions. One of these, which invokes the Coulomb interaction of Chl with charged amino acids in the protein, now appears most promising. We find that the Chl derivative, 3-desethyl-3-(aminomethyl) Chl a, exhibits a reversible 5-nm absorbance shift (to the blue) upon complete protonation of the amine nitrogen. Calculations by others strongly support this model, specifically that point charges selectively placed near the Chl periphery can induce redshifts of the magnitude observed in vivo, and also can have a large effect on the value of the Chl redox potential. We have also synthesized a Chl Schiff base that displays a reversible 23-nm redshift on protonation of the imine nitrogen. The possibility that a Schiff base linkage exists between Chl and an appropriate amino acid (e.g., lysine) in a photosynthetic protein complex is being explored for RC's of Rhodospeudomonas sphaeroides. Studies are planned with additional model compounds that have inducibly chargeable groups, and with techniques for exploring possible Chl-(charged-amino-acid) interactions in Chl-protein complexes from photosynthetic organisms.

3. BOYCE THOMPSON INSTITUTE
Cornell University, Ithaca, New York 14853

CARBON METABOLISM IN LEGUME NODULES — $40,034
Thomas A. LaRue

The objective of the project is to determine how the legume nodule uses carbohydrates to provide energy and reductant for nitrogen fixation. Because the plant cells within a nodule are essentially microaerobic, we are investigating the possible role of anaerobic pathways in metabolizing carbohydrates. We have established the utility of changing the gas phase available to bacteroids, detached nodules, or intact plants to manipulate enzyme activity. A brief treatment with pure oxygen decreases nitrogenase activity, and permits study of changes in processes closely related to nitrogenase. The oxidation and reduction of flavins and pyridine nucleotides in intact bacteria can be monitored *in situ* by changes in their fluorescence.

4. BRANDEIS UNIVERSITY
Waltham, Massachusetts 02254

EFFECT OF LIGHT ON RESPIRATION AND DEVELOPMENT OF PHOTOSYNTHETIC CELLS — $48,600
Martin Gibbs
Institute for Photobiology of Cells and Organelles

C.reinhardtii F-60, a mutant unable to fix CO_2, breaks down starch at an anaerobic rate of 12.4 $\pm$ 2.2 µmol glucose in starch consumed·mg^{-1}Chl·$4h^{-1}$. Light decreases the anaerobic rate by a factor of 2 and 4 at 40 and 100 w·m^{-2}. Fermentative products (moles) are, per mole of glucose consumed, in dark vs in light (100 w·m^{-2}): formate 1.8-2.1 vs 0.7-1.2; acetate 0.8-1.1 vs none; ethanol 0.8-1.0 vs 0.05-0.2; glycerol 0.02-0.06 vs 0-0.02; CO_2 0-0.15 vs 2.2-3.4; H_2 0.15-0.4 vs 6-6.8. Carbon recovery is 95-102% (dark) vs 60-75% (light); O/R index is 0.87-1.1 (dark) vs 0.67-1.05 (light); H recovery is 94-104% (dark) vs 65-84% (light). Starch breakdown rate is doubled by 5µM FCCP in dark, and reaches the dark level in light. Molar proportions of the fermentative products are not affected by FCCP in dark, except H_2 which is 0.1; in light, formate is 1.4-2.5, acetate 1.2-1.7, ethanol 0.1, CO_2 1.5-1.9, H_2 4-5.5. In light, 10µM DCMU decreases CO_2 and H_2 to (moles): 0.9-1.3 and 2.5-3.4, and increases formate to 1.5, while having no effect on the other products. Aerobically, ethanol and formate are not consumed in dark or in light. To account for the stoichiometry, the only known pathway is glycolysis followed by pyruvate breakdown into formate and acetyl-CoA. In dark, acetyl-CoA is converted to acetate and ethanol. Light (100 w·m^{-2}) redirects C and H flow since: 1) H_2 and CO_2 evolution is increased, 2) ethanol production is inhibited 3) acetate production is inhibited in absence of FCCP, 4) DCMU does not restore the pattern of fermentation seen in the dark. In addition, it is hypothesized that, in light, acetyl-CoA is converted to fatty acids except when FCCP is present, ethanol formation is prevented by light-induced inhibition of acetaldehyde dehydrogenase, and in the presence of DCMU H_2 formation results from reduced pyridine nucleotides preferentially feeding electrons to photosystem I.

5. UNIVERSITY OF CALIFORNIA AT SAN DIEGO
La Jolla, California 92093

HYDROGENASES, THEIR CLONING, PREPARATION, CHARACTERIZATION AND MODIFICATION FOR USE IN PHOTOBIOREACTORS — $75,000 (FY 82 funds)
Robert G. Bartsch, Martin D. Kamen and Nathan O. Kaplan
Department of Chemistry, A-002

We are seeking to characterize a hydrogenase molecule at the molecular level. The enzyme from Desulfovibrio vulgaris is readily crystallized from ammonium sulfate solution to yield crystals of sufficient size for initial x-ray crystallographic study. Because the enzyme proves to be unstable under the crystallization conditions tested we are studying alternate conditions which utilize low salt concentrations for generating suitable crystals. Based on two partial amino acid sequences with minimal degeneracy in the corresponding DNA sequences, we are synthesizing a mixture of all possible oligonucleotides which could code for the peptide fragments to serve as hybridization probes for identifying restriction enzyme generated gene fragments to be used to clone the hydrogenase gene and ultimately to determine the DNA sequence of the gene and consequently of the corresponding amino acid sequence of the gene product. From the x-ray crystallographic and amino acid sequence studies we propose to determine the three dimensional structure of the hydrogenase molecule. With the aid of this information we hope to be able to understand the enzyme mechanism for catalysis of the seemingly simple chemical reaction typified by the equation: $H_2 = 2H^+ + 2e^-$. Our long range goal is to learn how to incorporate a suitably engineered hydrogenase function into an organism such as a cyanobacterium in the effort to construct an active self-replicating fuel gas generator dependent on water and sunlight for raw materials. In a parallel study we have undertaken to identify possible suitable thermophilic cyanobacteria which might serve as a host for the proposed cell construct.

6. UNIVERSITY OF CALIFORNIA
Los Angeles, California 90024

ENERGY CAPTURE AND USE IN PLANTS AND BACTERIA — $82,000
Paul D. Boyer
Department of Chemistry and Biochemistry

Our studies focus on how plants use sunlight energy and bacteria use biomass energy to synthesize adenosine triphosphate (ATP). This is quantitatively the most prominent chemical reaction in the world. An ATP synthase complex in chloroplast and bacterial membranes forms ATP in a reaction sequence coupled to the use of an electrochemical proton gradient. Our laboratory has developed the energy-linked binding change hypothesis for ATP synthesis, in which identical catalytic sites on the enzyme participate in coordinated alternation. Experimental evidence favors the view that energy promotes competent binding of inorganic phosphate and adenosine diphosphate (ADP) at one catalytic site and the release of ATP from another. This mechanism appears to be gaining support but needs critical evaluation from many approaches. Studies are underway using ^{18}O-labeling probes of the reversal of bound ATP cleavage with the membrane-bound ATP synthase complex and the isolated CF_1-ATPase portion, and of the nature and extent of bound intermediates with ^{3}H and ^{32}P-labeled substrates. We will soon initiate fluorescent quench-flow studies of ATP and ATP analog binding. Together with earlier data the results may give a critical evaluation of the proposed existence of a transitorily tightly bound ATP that is rapidly and reversibly hydrolyzed at the catalytic site. Other studies underway arise from our new hypothesis that catalysis must be accompanied by a rotational reorientation of catalytic and noncatalytic subunits. As one probe of this we are studying selected chemical derivitization of subunits in the catalytic and noncatalytic state. Also, studies employing our ^{18}O-exchange techniques have been initiated with mutants forms of the E. coli enzyme with defective noncatalytic subunits to gain further insight on subunit interaction.

7. UNIVERSITY OF CALIFORNIA
Davis, California 95616

FLUORESCENCE PHOTOBLEACHING MEASUREMENTS OF PLANT MEMBRANE VISCOSITY: MECHANISMS OF RESISTANCE TO ENVIRONMENTAL STRESS — $60,000

R. W. Breidenbach, D. W. Rains, and M. J. Saxton
Plant Growth Lab/ Agronomy and Range Science

The purpose of this project is to examine the role of the plasma membrane in determining the responses of different crop species to temperature and salinity: two factors strongly limiting plant productivity. The experiments use fluorescence photobleaching recovery to compare the lateral diffusion rates of proteins and lipids in the plasma membranes of plants differing in their sensitivity to chilling temperatures or high concentrations of salts. Membrane viscosities of sensitive and resistant plants are being compared at various temperatures and salt concentrations. Since many important cellular processes may depend directly upon lateral motion of membrane proteins, this approach provides a direct measure of the relation between the physical properties of the membrane and plant responses to environmental stresses. Understanding of this relationship will provide useful strategies for developing tolerant new plant varieties for production of food, fuel and chemicals.

The techniques we are using will also enable us to examine two other problems in plant biophysics:

1) The effect of the cell wall on lateral diffusion rates
2) The mechanism by which certain polysaccharide fragments trigger the synthesis by the plant of defensive compounds against fungal attack.

8. UNIVERSITY OF CALIFORNIA
Berkeley, California 94720

THE REGULATION OF ENZYME SECRETION IN PLANT CELLS BY CALCIUM — $82,000

Russell L. Jones
Department of Botany

The objective of this project is to define the role of calcium in enzyme secretion from aleurone layers of barley (Hordeum vulgare L.) seeds. The Ca^{2+} concentration of the incubation medium regulates the release of two isozymes of α-amylase, as well as acid phosphatase, protease and ribonuclease from aleurone layers. Using pulse-labelling techniques in conjunction with electrophoretic and serological procedures, I propose to establish the relationship between enzyme synthesis and secretion in the presence and absence of Ca^{2+}. Cytoplasmic calcium levels will be determined with the fluorescent dye quin-2 in suspensions of barley aleurone protoplasts. Organelles involved in the sequestration of Ca^{2+} will be identified by light and electron microscopy. Chlorotetracycline fluorescence will be used to localize the sites of Ca^{2+} deposition in isolated protoplasts by light microscopy. For electron microscopy antimonate will be used to precipitate calcium as electron-dense calcium antimonate in aleurone layers incubated in the presence and absence of Ca^{2+}. Inhibitors of Ca^{2+} transport, Ca^{2+} antagonists and uncouplers will be used to interfere with Ca^{2+} sequestration and thus aid in the identification of those organelles involved in Ca^{2+} homeostasis. The presence of calmodulin in aleurone cells will be determined by extraction of this protein and identification of its activity via the activation of NAD kinase. The existence of other Ca^{2+}-binding proteins will be explored by measuring the Ca^{2+}-binding capacity of proteins purified by electrophoresis.

9. UNIVERSITY OF CALIFORNIA
Irvine, California 92717
Berkeley, California 94720

BIOENERGETICS OF SALT TOLERANCE — $135,000

James K. Lanyi
Dept. of Physiology and Biophysics, UC Irvine
Lester Packer
Dept. of Physiology and Anatomy, UC Berkeley

The bioenergetic aspects of cellular salt tolerance include ion transport across membranes, redirection of metabolic pathways for the increased synthesis of osmoregulatory compounds, replacement of some salt sensitive components with salt resistant ones, modification of the photosynthetic apparatus for increased efficiency, and the signals which turn these processes on and off during salt stress. We have developed and adapted methods to study these phenomena in three systems, each uniquely suited to answer specific questions. In membranes of Halobacterium halobium and the cyanobacterium, Synechococcus 6301, we are studying the active and passive transport of sodium, potassium, and chloride ions, and the regulation of the transporters. In whole cells of Synechococcus and in sugar beet (Beta vulgaris) leaf segments, we follow the pathway of carbon dioxide assimilation and the enzymes responsible before, during, and after growth in the presence of salt. In Synechococcus we explore the membraneous and cytoplasmic events which occur during short-term adaptation to salt. In thylakoids of Synechococcus and intact chloroplasts of sugar beet leaves, we are attempting to describe features of the photosynthetic apparatus which are changed by salt stress. Results with these systems so far have yielded interesting and promising results. Using this broad approach, we intend to develop the conceptual basis for a refined description of the physiology of cellular adaptation to salinity.

10. UNIVERSITY OF CALIFORNIA, LOS ANGELES
Los Angeles, California 90024

METHANOGENESIS FROM ACETATE, A KEY INTERMEDIATE IN NATURE — $85,974 (14 months)

Robert A. Mah
Division of Environmental & Nutritional Sciences

The objective of this project is to isolate and characterize new strains and species of methane-producing bacteria, particularly those responsible for converting acetate to methane and carbon dioxide. The approach utilizes samples from anaerobic habitats inoculated into an acetate enrichment system. Sediment from the La Brea Tar Pits, Los Angeles, Ca., a solar saltern, a swine waste lagoon, and a peat bog were examined. Methane evolution was followed by gas chromatographic measurement of the head space. When methane was formed at an exponential rate, a roll-tube dilution of the enrichment is made into habitat-simulating media containing acetate, methanol, or trimethylamine but not H_2. Colonies exhibiting fluorescence under UV epi-illumination are picked and purified. We are characterizing three isolates from these samples. Two of these are hydrogen-oxidizing methanogens which exhibit differences in cationic requirements and/or immunological cross reactivity sufficient to warrant further scrutiny as new species. The third isolate is a halophilic methylotroph which utilizes methanol and trimethylamine but not acetate nor H_2/CO_2 as methanogenic substrates. This latter isolate appears to be widely distributed in hypersaline environments of marine origin. Further characterization of physiological, morphological, and macromolecular properties of these isolates is ongoing.

11. UNIVERSITY OF CALIFORNIA AT SAN DIEGO
La Jolla, California 92093

SELECTION OF MUTANTS INCREASING THE RATE OF FERMENTATION IN YEAST — $50,000
Christopher J. Wills
Department of Biology, C-016

We are using a variety of selective approaches to investigate the role in yeast metabolism of energy transfer mechanisms across the mitochondrial membrane, most particularly in the regulation of glycolysis and gluconeogenesis. An understanding of this regulation will in turn enable us to select yeast strains with greatly increased metabolic rates.

Our primary approach is to select for mutants that can grow well under conditions in which the transfer of energy-rich compounds across the mitochondrial membrane is limiting. One of these conditions is growth on a simple medium with glycerol as a sole carbon source. Mutants able to grow on this medium have apparently increased the efficiency of the malate-aspartate shuttle, one of the shuttles involved in regulating the flow of energy across the membrane. Other shuttles and transport systems are also susceptible to mutational alteration, through growth on limiting media in the presence of various inhibitors. In addition to examining these mutants for altered metabolism, we will screen for altered mitochondrial membrane proteins. Isolation of these latter mutants will enable the genes for these proteins to be cloned, and increase our knowledge of the molecular basis of mitochondrial membrane transport.

12. UNIVERSITY OF COLORADO
Boulder, Colorado 80309

STUDIES OF PLANT CELL WALLS AND OF PLANT-MICROBE INTERACTIONS — $300,000
Peter Albersheim, Alan G. Darvill, Michael McNeil and Barbara Valent
Department of Chemistry, Campus Box 215

The DOE grants support four major projects in this laboratory. These are: identifying, isolating, and characterizing naturally occurring carbohydrates with biological regulatory functions, developing new methods for the purification and structural characterization of complex carbohydrates, delineating the structures of the polysaccharides present in the walls of growing plant cells, and developing a genetic system for Pyricularia oryzae, the fungus that causes rice blast disease. The latter project has, as its primary goal, the identification of the genes and gene products responsible for race and cultivar specificity in this host-pathogen system. All of these projects, but especially the first three, are closely interrelated. Using newly developed techniques, many of which are being developed in our laboratory, for the purification and structural characterization of complex carbohydrates, we have discovered that the carbohydrates that comprise the plant cell wall are far more structurally complex than had been envisioned. A question that we are attempting to answer is why are these cell wall polysaccharides so complicated. A possible answer comes from our observation that plant cell wall oligosaccharides, when released from the confines of the cell wall, appear to regulate a variety of physiological functions in plants, such as morphogenetic differentiation, growth rate, and defense against pathogens.

13. CORNELL UNIVERSITY
Ithaca, New York 14853

STUDIES OF PHOTOSYNTHETIC ENERGY CONVERSION — $65,000
Roderick K. Clayton
Division of Biological Sciences

We continue to study the photochemical and associated "dark" reactions of photosynthetic bacteria; principally Rhodopseudomonas sphaeroides and Rp. viridis. Our methods include optical absorption and emission spectrometry, measurements with polarized lights, and some specialized spectrometric techniques (EPR, Raman and atomic absorption). We continue to explore the reversible binding of the 800 nm component of the B850 antenna pigment protein in Rp. sphaeroides. Our aim is to learn the nature of the bacterial chlorophyll-protein binding, especially through the competitive binding of bacterial chlorophyll and related molecules. To aid in these studies we have developed a laboratory computer system based on the HP9826 computer.

14. CORNELL UNIVERSITY
Ithaca, New York 14853

EFFECTS OF FREEZING AND COLD ACCLIMATION ON THE PLASMA MEMBRANE OF ISOLATED CEREAL PROTOPLASTS — $42,017
Peter L. Steponkus
Department of Agronomy

The primary objective of the project is to characterize the stress-strain relationship (SSR) of non-acclimated (NA) and acclimated (ACC) protoplasts (Secale cereale L. cv. Puma) to provide a mechanistic basis for the increased tolerance of acclimated protoplasts to large area deformations and; as a result, the decreased incidence of expansion-induced lysis during a freeze-thaw cycle. The large difference in the tolerable surface area increment between NA and ACC protoplasts is the result of differences in the subduction/incorporation of membrane material during contraction/expansion and is not attributable to differences in the elastic properties of the plasma membrane. Whereas in-NA protoplasts osmotically induced contraction results in deletion of membrane area by endocytotic vesiculation, contraction of acclimated protoplasts results in the exocytotic extrusion of membrane material that remains contiguous with the plasma membrane. Material subducted into endocytotic vesicles in NA protoplasts is not as readily reintroduced into the plasma membrane as is the material which is exocytotically extruded in ACC protoplasts. As a result, the proportional rate of change in area as a function of tension, $Z(\gamma)$, is substantially higher in ACC protoplasts during expansion following hypertonic-induced contraction. In contrast, $Z(\gamma)$ of NA protoplasts is similar whether the protoplasts are expanded from hypertonic or isotonic solutions. Partial conservation of membrane material in osmotically contracted ACC protoplasts results in a lower, possibly even zero, resting tension (γ_r) in contrast to the reestablishment of γ_r in NA protoplasts. Freeze fracture analysis demonstrates that the protein complement of the PF_p fracture face of the plasma membrane is conserved due to the formation of crystalline arrays and the preferential deposition of lipid material in the interior of the exocytotic extrusions.

15. CORNELL UNIVERSITY
Ithaca, New York 14853

THE IMPORTANCE OF PHYTOALEXIN TOLERANCE AND DETOXIFICATION FOR PATHOGENICITY — $38,377

Hans D. VanEtten and David E. Matthews
Department of Plant Pathology

The production of antimicrobial compounds (phytoalexins) by plants is believed to function as an active mechanism of disease resistance which is effective against at least some microorganisms. However, phytoalexin-producing plants are nonetheless susceptible to some diseases. Our research has indicated that one way in which successful pathogens can overcome this resistance mechanism is by detoxifying their hosts' phytoalexins. The primary host-parasite interaction we have investigated is a root and stem rot disease of pea (Pisum sativum) caused by the fungus Nectria haematococca (Fusarium solani). Virulent isolates of this fungus detoxify pisatin, the major phytoalexin produced by pea. Genetic studies involving crosses between appropriate isolates strongly suggest that the ability to detoxify pisatin is an essential trait for virulence on this host. The detoxification reaction is catalyzed by a substrate-inducible cytochrome P-450 monooxygenase. N. haematococca detoxifies at least two other phytoalexins produced by other legume species of which it is a pathogen. These reactions are also mediated by oxygenases. The objectives of this research proposal are to characterize further the enzymes responsible for phytoalexin detoxification, especially with regard to their substrate specificity, sensitivity to inhibitors, regulation, and relationship to virulence. Both biochemical and genetic analyses will be used to accomplish these objectives. The results will have significance for potential practical applications involving phytoalexins as a means of disease control, as well as for basic theories of plant-parasite interactions.

16. CORNELL UNIVERSITY
Ithaca, New York 14869

MICROBIAL ECOLOGY OF THERMOPHILIC ANAEROBIC DIGESTION — $68,083

Stephen H. Zinder
Department of Microbiology

The anaerobic digester is a microbial ecosystem in which several groups of microorganisms must interact effectively if efficient bioconversion of organic matter to methane is to occur. Our understanding of the organisms involved in anaerobic digestion and their interactions is still rudimentary. The objective of this project is to provide an integrated understanding of the ecology of the microbial populations present in a thermophilic (58°C) laboratory-scale digester being fed a lignocellulosic waste. To do this we have used cultural, microscopic, and radiotracer techniques. We have been especially interested in the ecology of methanogens in the digester. Results obtained thus far include: (1) the discovery and isolation of a two-membered microbial coculture which converts acetate to methane via interspecies hydrogen transfer rather than the aceticlastic reaction; (2) the discovery of a thermophilic Methanothrix. This organism has not been described previously and grows at temperatures over 65°C, contains gas vacuoles, and grows more rapidly than mesophilic strains; (3) Methanothrix eventually displaced Methanosarcina as the dominant aceticlastic methanogen in the digester, possibly because of its low K_s value for acetate (0.3 mM); (4) When Methanosarcina, which does not grow at 65°C, was dominant in the digester, an upwards temperature shift to 65°C caused acetic acid buildup and digester failure. When Methanothrix was dominant, the temperature shift did not inhibit methanogenesis from acetate; (5) Methanogenesis from acetate in the digester was completely inhibited by 1 mM 2-bromoethanesulfonate (BES) while 50 mM BES was required for inhibition of methanogenesis from CO_2. Thus, toxicants can affect aceticlastic and CO_2 reducing methanogenic populations differently.

17. FLORIDA STATE UNIVERSITY
Tallahassee, Florida 32306

GUARD CELL BIOCHEMISTRY: RESPONSES TO ENVIRONMENTAL STIMULI CAUSING CHANGES IN GAS EXCHANGE — $74,655

William Outlaw
Department of Biological Science

The objective of this project is to investigate guard cell biochemistry, particularly as it is affected by the environment. (Guard cell pairs, or "stomata", are sprinkled throughout the surface of leaves. Each pair resembles a donut, except the pore size is adjustable, depending on the turgidity of the surrounding guard cells. Virtually all CO_2 for photosynthetic reduction enters the leaf through these pores; likewise, water loss from the leaf also passes through these pores. Thus, the function of these cells is to control gas exchange. Several environmental variables are integrated to optimize aperture size.) Our approaches to this problem are diverse; a particular difficulty is to obtain sufficient quantities of these cells in pure form. One approach is the isolation of guard cell protoplasts. Although we do not have the techniques perfected, we have published one paper on purification of enzymically released cells. Our second approach is to dissect out individual cell samples, which may be subsequently assayed using either quantitative histochemical methodology (one paper on carbon metabolism) or other sensitive techniques (quantification of the phytohormone, ABA). Our third approach is to optically isolate cells. Using this approach, we have unequivocally localized PSII in guard cells (published). In addition, a review article on the role of potassium in guard cell has been submitted; this review complements my recent review on carbon metabolism in these cells.

I hope our work will have practical implications. Production of much of the food, fiber and shelter in this country relies on the functioning of these cells. As important, a better understanding of the regulation of water loss from plants may provide opportunities to conserve this limiting resource.

18. UNIVERSITY OF FLORIDA
Gainesville, Florida 32610

INVESTIGATION OF THE TRANSPOSITION OF MITOCHONDRIAL DNA AND ITS RELATIONSHIP TO FERTILITY IN *ZEA MAYS* — $68,961

Rusty J. Mans
Department of Biochemistry and Molecular Biology,
J-245, JHMHC

We are looking for altered expression of mitochondrial genes that affect male fertility in maize. These genes are rearranged and their copy numbered altered upon the spontaneous reversion of an S-type cytoplasmically male sterile parental plant to fertility. Sterility in these lines is also suppressed or repressed by the dominant allele of a nuclear gene, *i.e.* restorer to fertility (Rf3). We have cloned segments of the transposable mitochondrial genes into pB R322 for use as templates in an *in vitro* transcription system. We have purified an alpha-amanitin sensitive RNA polymerase from maize seedlings that preferentially transcribes cloned DNAs. We will characterize the RNA products accumulated in the system as to size and nucleotide sequence. By comparison of transcripts of appropriate cloned segments of the mitochondrial genome from sterile and fertile revertant plants we will detect altered transcription as a consequence of gene rearrangement in plant mitochondria. These results will facilitate the use of portions of the mitochondrial genome as putative vehicles for genetic engineering of this agronomically important grain.

19. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

ROLE OF Ca^{2+} AND CALMODULIN IN PHOSPHORYLATION IN PLANTS — $50,000
Milton J. Cormier
Department of Biochemistry

The long term objectives are to better understand the role of Ca^{2+} and calmodulin in cellular regulation in plant cells. The short term objective is to understand the role of Ca^{2+}-dependent phosphorylation in plant cells. Our demonstration of the presence of high affinity Ca^{2+} binding proteins (such as calmodulin) in plants strongly suggest that free Ca^{2+} is acting as a second messenger in plant cells. Our recent observation that Ca^{2+} and calmodulin are absolute requirements for the activation of plant NAD kinase provide further support for this theory. These findings suggest that free Ca^{2+} may be important in mediating some of the plant responses to stimuli such as light, auxins, gibberellins, and cytokinins. We are examining the Ca^{2+}-dependent regulation of phosphorylation, i.e. phosphorylation of small molecules (such as NAD) and proteins. We are examining these regulatory events in several soybean tissue culture cell lines. Studies on these broad based regulatory functions of calmodulin in plants may lead to the formulation of new growth regulators, new herbicides, and the manipulation of flowering time.

20. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

BIOSYNTHESIS OF A MICROBIAL BIOSURFACTANT: A NOVEL AND UNIQUE PRODUCT — $75,000
W. R. Finnerty
Department of Microbiology

The objective of this project is to determine the mechanism of biosynthesis of a microbial-produced extracellular glycolipid biosurfactant which is effective in the viscosity reduction of heavy crude oil. The approach is to study the enzymology of glycolipid biosynthesis and the genetic relationship between alkane utilization and glycolipid synthesis. Results to date show the glycolipid can be labeled with specific radioactive precursors: glycerol, acetate, propionate, glucose and palmitate. Acyl transacylase activity has been localized in the soluble fraction which acylates the water-soluble backbone of the glycolipid. Glycolipid is synthesized only by alkane-grown cells. The microorganism contains three plasmids of 55, 14.5 and 11.5 Mdal. The genetic and metabolic relationship between alkane utilization and glycolipid formation will be determined. The glycolipid forms stable oil-in-water microemulsions of heavy crude oils with significantly improved rheological properties in the oil. Such bioproducts have application to the microbial desulfurization of high-sulfur crude oil, transportation of heavy oils and enhanced oil recovery.

21. UNIVERSITY OF GEORGIA
Tifton, Georgia 31793

DEVELOPMENT OF INNOVATIVE TECHNIQUES THAT MAY BE USED AS MODELS TO IMPROVE PLANT PERFORMANCE — $36,000

Wayne W. Hanna and Glenn W. Burton
Department of Agronomy

The objectives of this project are to develop techniques for transferring genes from wild species to cultivated plant species, to demonstrate the wealth of germplasm in the secondary and tertiary gene pools that can be transferred to cultivated species and to develop an obligate apomictic pearl millet. Species within the genus Pennisetum are being used as test organisms. The approach utilizes plants of wild species with different genetic backgrounds and ploidy levels (chromosome numbers) crossed and backcrossed with different genotypes of pearl millet, P. americanum, with different ploidy levels to produce fertile interspecific hybrids and derivatives. Germplasm is being transferred to pearl millet through genetic recombination in the interspecific hybrids followed by genome segregation, only genome segregation, and/or by using gamma radiation to produce small translocations (chromosomes with desirable genes) between chromosomes of the wild species and pearl millet. These studies are providing valuable information on the most efficient ways to transfer alien germplasm and could result in the transfer of valuable genes such as pest resistance, drought tolerance, perennial growth habit and apomixis to pearl millet. The overall impact would be on increased, more efficient and more reliable production of food, fiber, and forage.

22. UNIVERSITY OF GEORGIA
Athens, GA 30602

ENVIRONMENTAL STRESS MEDIATED CHANGES IN TRANSCRIPTIONAL AND TRANSLATIONAL REGULATION OF PROTEIN SYNTHESIS IN CROP PLANTS — $84,000

Joe L. Key
Department of Botany

When seedlings of soybean, and a wide range of other crop plants, are subjected to a temperature shift from 28°-30° to about 40° (heat shock or hs), there is a rapid and dramatic shift in the pattern of protein synthesis. Plants synthesize 30 to 40 hs proteins and greatly reduce normal protein synthesis during hs. These hs proteins seem to provide thermal protection to the plant; that is, plants subjected to a tolerant hs temperature (e.g. 40° for soybean) for some 2-3 hr are now tolerant of an otherwise lethal temperature (e.g. 45° for 2 hr). A number of treatments lead to the development of thermal tolerance in soybean: 1) 40° for 2 hr, 2) 45° for 4 to 8 min followed by 2 hr at 28°, 3) gradual increase in temperature (e.g. 3° per hr) from 30° up to 45°-47.5° and 4) arsenite (50 um) for 2 to 4 hr, a treatment resulting in a fairly common pattern of hs protein synthesis. Thermal protection appears to relate to selective cellular localization of some of the hs proteins during hs.

Cloned cDNAs have been used in an analysis of hs mRNA synthesis. Following hs at 40° to 42°, hs mRNAs are detected within 3 to 5 min; they accumulate for about 2 hr up to levels of 20,000 copies per cell. A shift back to 28° results in a loss of mRNAs with a 1/2 time of about 1 hr. There is a gradual decline of mRNA levels after about 4 hr of continuous 40° hs. A 4 to 10 min hs at 40° results in transient and low level accumulation of hs mRNAs while a 4 to 10 min hs at 45° results in accumulation of hs mRNA over the next 4 to 6 hr at 28° to levels similar to a 2 to 4 hr hs at 40°.

Of physical stresses studied to date (e.g. water stress, anaerobiosis, high levels of hormones, heavy metals), arsenite most nearly mimics hs, though these stresses result in accumulation of detectable levels of hs mRNAs. One set of hs mRNAs (for 4-5 27 kD proteins) which, in contrast to other hs mRNAs, is present in unstressed tissue, is induced to hs levels by such stresses.

23. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

SOYBEAN RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT GENE FAMILY: GENE STRUCTURE AND REGULATION OF GENE EXPRESSION — $70,000

Richard B. Meagher
Department of Molecular and Population Genetics

Genetic engineering systems in bacteria and in animal cells have made use of well characterized homologous promoter/regulator sequences to control foreign gene expression. It is likely that similar plant control sequences can be used to control foreign gene expression in transformed plant cells. The ribulose bisphosphate carboxylase gene family in soybean is ideally suited to examine strong transcriptional control signals in plants. The gene family is highly diverged and only functionally related regions of DNA would be expected to share homologous DNA sequences. We have completely sequenced one soybean small subunit gene, partially characterized the light induced level of its transcription and identified potential transcriptional control sequences. Furthermore, we have partially characterized the soybean small subunit gene family and shown that it contains several members. We propose to characterize the small subunit gene promoter/regulator sequences in order that they might be used to control foreign gene expression in plant cells. As part of this project we plan to isolate, characterize, and sequence most of the RuBP carboxylase small subunit gene family members in soybean, determine if their mRNA levels are light regulated and if this is due primarily to transcriptional regulation, identify the 5' and 3' ends of their mRNA products, and compare potential homologous promoter/regulator sequences. Quantitative evolutionary measurements will be made in order to determine the degree of divergence of small subunit genes within soybean. Various regulatory elements from the small subunit gene could then be used for transcriptional control of foreign genes manipulated into plants.

24. UNIVERSITY OF GEORGIA
Athens, GA 30602

THE MICROBIOLOGY AND PHYSIOLOGY OF ANAEROBIC FERMENTATIONS OF CELLULOSE — $240,000

H. D. Peck, Jr., and L. G. Ljungdahl
Department of Biochemistry

Investigations into the biochemistry and physiology of the four major groups of microorganisms (primary, ancillary, secondary and methane bacteria) involved in the anaerobic conversion of cellulose to methane and carbon dioxide will be continued. Studies on the primary or cellolytic microorganisms will be focused on the isolation of new thermophilic strains from Iceland, interactions with ancillary bacteria which ferment cellobiose and xylose, growth and modification of fermentation patterns by inorganic pyrophosphate and purification of cellulase. The projected investigations of the ancillary bacteria will emphasize isolation of new strains and increasing ethanol production with T. ethanolicus. The latter research will involve genetic modifications, enzymological studies on the regulation of appropriate enzymes and a study of the effect of inorganic pyrophosphate on growth and fermentation patterns. The enzymology of acetate formation from carbon dioxide by acetogenic bacteria will be studied with initial emphasis on the metabolism of the one-carbon compounds. Further studies with these organisms will include bioenergetics, especially hydrogen metabolism and energy coupling by H_2 cycling, and the structure and function of electron transfer components. Research on secondary bacteria will emphasize the sulfate reducing bacteria from the aspects of H_2 cycling, specificities of electron transfer proteins and enzymes, the mechanism of bisulfite reductase and APS reductase and the enzymology and physiology of new genera of sulfate reducing bacteria. The biochemistry and physiology of both H_2-utilizing and acetate utilizing methanogens will continue to be investigated. The studies with H_2-utilizing methanogens will stress hydrogenase and the effect of inorganic pyrophosphate on growth. The research on the acetate-utilizing methanogens will involve the bioenergetics of sulfite reduction and the mechanism of acetate formation induced by pyrophosphate.

25. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

PHYTOCHROME PROPERTIES AND FUNCTION IN PHOTOSYNTHETICALLY COMPETENT PLANTS — $47,588
Lee H. Pratt
Department of Botany

Phytochrome is a chromoprotein that senses the wavelength distribution of incident light energy and responds to it by modulating the growth and development of green plants. The objective of this program is to characterize phytochrome as it exists in photosynthetically competent plants and to help understand how it influences photosynthetic productivity. This work depends heavily upon application of immunochemical methods for three reasons. (1) The chlorophyll in green plants makes unsuitable the widely used spectrophotometric assays for phytochrome. (2) So little phytochrome is present in green tissues that spectrophotometric assays are generally too insensitive. (3) Antibodies increase greatly the ability to probe the structure and function of a complex molecule such as phytochrome. To ensure maximum specificity and utility of immunochemical approaches, monoclonal antibodies to both pea (Pisum sativum L.) and oat (Avena sativa L.) phytochrome are being produced. These antibodies are in use to quantitate phytochrome in crude extracts from green plants at the femtomol level, to probe the structure of phytochrome as it is isolated from green plants, and to determine the distribution and subcellular localization of phytochrome by immunocytochemistry. Phytochrome in and from both peas and oats is being investigated to determine whether information obtained is of general applicability or is perhaps specific to only one plant or one group of plants. Knowledge deriving from this work will not only help clarify the general question of how phytochrome regulates light-mediated plant growth and development but also the more specific question of how it influences the efficiency with which plants convert solar to chemical energy.

26. HARVARD UNIVERSITY
Cambridge, Massachusetts 02138

UNRAVELING PHOTOSYSTEM II — $76,815
Lawrence Bogorad
Department of Cellular and Developmental Biology

The objective of this project is to identify and characterize genes involved in photosynthesis, particularly photosystem II, by a study of cyanobacteria. The two principal approaches being employed to identify genes for components of photosystem II in cyanobacteria. One is by using antibodies generated against a photosystem II preparation to identify those E. coli strains transformed with a library of cyanobacterial DNA that carry genes for photosystem II components. Another approach is through the use of maize chloroplast genes that hybridize to cyanobacterial DNA as heterologous probes.

27. HARVARD UNIVERSITY
Petersham, Massachusetts 01366

STRUCTURE AND FUNCTION OF FRANKIA VESICLES BY DINITROGEN FIXATION OF ACTINORHIZAL PLANTS — $42,770

John G. Torrey and John D. Tjepkema
Cabot Foundation, Harvard Forest

In root nodules of symbiotic dinitrogen-fixing trees, the actinomycetous endophyte Frankia forms terminal swellings or vesicles which are believed to be the site of the enzyme nitrogenase. When isolated and grown in synthetic culture media lacking combined nitrogen, Frankia also differentiates vesicles and fixes N_2. In our studies we have defined the chemical and physical conditions maximizing vesicle formation and acetylene-reducing (=nitrogenase) activity. Cells are grown in 3-l air-sparged magnetically stirred cultures with doubling time <24 hr. Growth is estimated by protein assay. Maximum acetylene reduction rates are obtained with 5 mM propionate as sole C-source, at pH 6.7 and 28°C. Frankia fixes N_2 under aerobic conditions and our studies have focussed on the mechanisms for O_2 protection of the nitrogenase enzyme. Evidence from kinetic analysis of in vivo enzyme rates suggests a passive gas diffusion barrier. Comparison of O_2 consumption rates in undifferentiated and vesicle-containing cells suggests also a form of "respiratory protection". Further studies of vesicle structure at the light and EM levels are being pursued in the effort to correlate structure with function.

28. THE HELICON FOUNDATION
San Diego, California 92121

CONSTRUCTION AND ANALYSIS OF BACTERIAL STRAINS USEFUL IN CONVERSION OF CELLULOSE TO ETHANOL — $59,722 (FY 82 funds)

Richard W. Armentrout

We will use recombinant DNA technology to construct a plasmid DNA suitable as a cloning vector for Zymomonas mobilis. This vector will be used to transfer genes from E. coli by mating. The expression of various genes which are active in E. coli will be examined in Zymomonas, including the gene for cellobiose utilization. Libraries of cloned DNA fragments from the gram negative cellulose utilizing organism Cellvitrio vulgaris will be screened to identify genes involved in cellulose degradation. These steps are preliminary to the construction of a set of genes which will function in Z. mobilis and allow us to examine a minimal gene set for bacterial cellulose degradation.

29. UNIVERSITY OF IDAHO
Moscow, Idaho 83843

GENETICS AND CHEMISTRY OF LIGNIN DEGRADATION BY STREPTOMYCES — $87,500
Don L. Crawford
Department of Bacteriology and Biochemistry

The objectives of this project are to develop and utilize protoplast fusion and protoplast transformation as recombinant DNA techniques for genetic improvement of lignin degrading Streptomyces, and to characterize the chemical changes in the structure of lignin resulting from the expression of specific lignin catabolism genes. The approach utilizes three lignin degrading Streptomyces strains which differ from one another in their ligninolytic activities and in aromatic compound catabolizing abilities. Protoplast fusion will be utilized to obtain recombinants expressing desirable traits derived from two or more parental strains. Stable lignin degradation enhanced mutants will be isolated and characterized. Genes coding for catabolism of selected aromatic compounds, or for degradation of lignin, will be transformed into protoplasts of other lignin-degrading or nonlignin-degrading strains, and transformants will be characterized to determine how expression of the added genes affects lignin degradation. The technique may be useful in determining the minimum number of genes required for lignin degradation in Streptomyces. Concomitantly, the chemical changes in lignin and the formation of lignin degradation intermediates resulting from degradation will be monitored, and recombinant organisms will be compared with the wildtype parental strains to determine how specific genetic changes affect the catabolic pathway.

30. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

FATTY AND AROMATIC ACID CATABOLIZING BACTERIA IN METHANOGENIC ECOSYSTEMS — $57,354
Marvin P. Bryant
Department of Dairy Science

In complete anaerobic degradation of organic matter to CH_4 and CO_2, three metabolic groups of bacteria are mainly involved; (1) hydrolyzing and fermentative bacteria, (2) obligate proton-reducing acetogens and (3) acetate, methanol, formate and H_2-CO_2-using methanogens. Group 2, includes syntrophs which require methanogens or other H_2-using bacteria to maintain a low concentration H_2 in the ecosystems in order to degrade certain organic compounds. Syntrophomonas β-oxidizes short-chain fatty acids to acetate (or acetate plus propionate) and H_2. Syntrophobacter degrades propionate to acetate, CO_2 and H_2 or formate. In the present work, Syntrophus, which catabolizes benzoate and, probably, hydrocinnamate, to acetate, CO_2 and H_2 and/or formate in association with an H_2-user has been documented. Other syntrophs, one catabolizing phenylacetate, and phenol and, probably, benzoate and hydrocinnamate; and another morphotype catabolizing phenol (other phenolics not yet studied) have been isolated in co-culture with H_2-using Desulfovibrio and with Wolinella (H_2 + fumarate to succinate). A long-chain fatty acid-degrading syntroph from stearate enrichment has been isolated in co-culture with Desulfovibrio using tridecanoate as energy source. The culture contains small amounts of a sugar-fermenting contaminant which does not catabolize fatty acids. The fatty acid-degrading bacterium is similar to Syntrophomonas in morphology and catabolizes butyrate, tridecanoate, stearate and, probably, other saturated fatty acids other than acetate, propionate and isovalerate. It is being purified of the contaminant before further studies are done. These studies add to basic knowledge of methanogenic ecosystems.

31. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

PHOTOSYNTHESIS IN INTACT PLANTS — $116,000
A. R. Crofts
Department of Physiology and Biophysics

In the intact plant, the photochemical reactions, and the reactions of electron transfer and proton transport which they drive, are part of an integrated mechanism which responds to the physiological state of the plant as this is determined by environmental factors. Rates of electron transfer, and the control of cyclic and non-cyclic pathways, can be assayed directly by following the changes on illumination of redox components of the chain, using spectrophotometry, or indirectly using fluorescence techniques. The generation and utilization of the proton gradient can be assayed by following the 515 nm electrochromic change. Our research is aimed at developing instrumentation to facilitate such measurements. A major initial emphasis has been on laboratory-based research designed to develop and test prototype instruments, and to understand in a controlled environment the factors determining the kinetic events we can monitor instrumentally. Our major effort has been on the mechanism of the two-electron gate by which PS II delivers electrons to the plastoquinone pool, but we have also studied reactions on the donor side of PS II with a view to defining conditions for isolating the reactions of the secondary donor Z so that we can characterize its absorption spectrum.

The instruments developed or in prototype include a rapid kinetic fluorimeter; dual-flash kinetic fluorimeter; computer-linked fluorescence induction fluorimeter; kinetic spectrophotometer with flash measuring beam; and kinetic spectrophotometer for measuring pseudo-steady-state kinetics. Three of these instruments are being developed in portable form, and are designed for field use.

32. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

MECHANISM OF PROTON PUMPING IN BACTERIORHODOPSIN — $51,971
Thomas G. Ebrey
Department of Physiology and Biophysics

The purple membrane of Halobacterium halobium probably represents the simplest biological solar energy conversion system. Light absorbed by bacteriorhodopsin, a small protein whose chromophore is retinal, directly leads to the transport of protons across the cell membrane. The resulting chemiosmotic potential can be used to make ATP. An additional feature of the purple membrane is its ability to pump protons over a wide variety of salt concentrations including in extreme saline environments. This proposal is to investigate the relationship between the transport of protons across the membrane and structure and conformation of bacteriorhodopsin. We have made an especially intriguing discovery, that the number of protons released by purple membrane sheets by light can be drastically altered by the proteolytic removal of a few amino acids from the C-terminal "tail" of bacteriorhodopsin. Thus we believe that we have a way of specifically controlling the release of some of the protons by altering a small part of the polypeptide chain. In addition the number of protons released has been shown to be a function of the salt concentration, which may in turn affect the protein conformation. We suspect this effect may be localized to the interaction of the C-terminal end of bacteriorhodopsin with the rest of polypeptide. This proposal centers around a set of experiments, based on these observations, to correlate the structure of the purple membrane with its energy transducing function.

33. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

DEVELOPMENT OF A GENETIC SYSTEM FOR BACTEROIDES SPECIES — $63,035
Jeffrey F. Gardner, Abigail A. Salyers
Department of Microbiology

The objective of this project is to develop a method for introducing DNA into Bacteroides. We have constructed a chimeric plasmid (pEG1) which contains a cryptic Bacteroides plasmid (from B. eggerthii B8-51) and pBR328 from E. coli. We have used this chimeric plasmid to test a number of transformation procedures including spontaneous uptake, calcium shock and spheroplasting. Recipients included not only cured B8-51 but also strains of other colonic Bacteroides species. No transformants were detected. We also attempted to transfer pEG1 from E. coli to Bacteroides. P plasmids of E. coli mobilized pEG1 from E. coli to E. coli at high frequency, both aerobically and anaerobically. However, when E. coli was mated with Bacteroides, under a variety of conditions, no transconjugants were obtained. Since it is possible that the selectable markers on pBR328 are not expressed in Bacteroides, we have cloned DNA from B. fragilis which complements trpE in E. coli. This DNA has been inserted in pEG1 to form a new plasmid (pEG100). We will isolate an appropriate auxotroph of B. fragilis to serve as a recipient for pEG100. We will use this strain and pEG100 to test various transformation procedures and conjugation conditions. To aid us in checking mutants and classifying natural isolates, we have developed a method for using cloned DNA fragments to identify colonic Bacteroides. This method could be very useful to a number of workers because procedures normally used to identify colonic Bacteroides species, on the basis of phenotypic traits, are cumbersome and time consuming.

34. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

BIOCHEMICAL AND BIOPHYSICAL STUDIES ON THE E. COLI AEROBIC RESPIRATORY CHAIN — $90,000
Robert B. Gennis
Departments of Chemistry and Biochemistry

Bacteria use a mechanism similar to mitochondria and chloroplasts to conserve energy and convert it to a usable chemical form. In particular, a transmembrane "proton motive force" is generated concomitant with electron flow through an electron transport chain. We are studying the components in the E.coli membrane responsible for generating this electrochemical gradient. E. coli has been selected because of the relative ease with which genetics can be applied to the problem, and also because of the apparent simplicity of the electron transport chain. We are emphasizing the coordinate application of biochemical, immunological and genetics techniques to identify and characterize each component of the aerobic respiratory chain. Our attention has focussed on the cytochrome d terminal oxidase complex which we have recently purified and reconstituted in an artifical, energy-conserving liposome system. Our attentions will now focus on the cytochrome o complex, about which much less is known. We have immunologically characterized this and demonstrated that it contains two b cytochromes, 4 polypeptide subunits, and functions as a "coupling site" or point of proton translocation in the membrane.

35. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

THE ROLES PLAYED BY MITOCHONDRIAL DNA PLASMIDS AND NUCLEAR GENES IN REVERSIONS TO FERTILITY IN S-TYPE MALE-STERILE MAIZE — $72,000

John R. Laughnan
Department of Genetics and Development

These investigations are concerned with the genetic and molecular basis of cytoplasmic male sterility and involve field and laboratory studies of special strains of maize. In particular, genetic reversion from the male-sterile condition to male fertility, the normal condition, is being investigated. Such reversions may occur at the cytoplasmic or nuclear level. Cytoplasmic reversion is associated with disappearance of the S-1 and S-2 mitochondrial DNA plasmids and has been shown to involve transpositional events within the mitochondrial genome. With collaborators we have experiments underway to determine whether the nuclear revertants have a similar basis. We have shown recently that maize nuclear DNA shares some DNA sequences with those of the S-1 plasmid in the mitochondrion. When reversion to fertility occurs at the nuclear level it is associated with transpositional insertion of fertility elements at one or another site within the chromosomal complex, and such elements may undergo secondary transposition to other chromosomal positions. Aspects of this secondary transposition phenomenon are being investigated. Developmental studies of the cytoplasmic reversion event are also being carried out. Since loss of the S-1 and S-2 mitochondrial DNA plasmids is associated with cytoplasmic reversion, but is not instantaneous, analysis of mitochondrial DNA in tissues of revertant plants, and their offspring, offers the opportunity to trace a developmental happening at the molecular level. Certain revertants from male-sterility conditions to male fertility are associated with failure of male-gametophyte or pollen function, but are unimpaired in female transmission. Since it appears that these reversion events involve a research sequence event, and that different chromosomal target sites are involved, they probably represent selected events in which insertions have occurred within genes essential for male-gametophyte function. We have intensified our studies of these revertants since they provide the first opportunity to identify and map genes affecting male gametophyte (pollen) function in maize.

36. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

ACETOPHILIC METHANOGENIC CONSORTIA — $85,000 (FY 82 funds)

Ralph S. Wolfe
Department of Microbiology

The purpose of this research program is to study microbes that participate in the anaerobic degradation of organic matter to acetic acid and of the conversion of acetic acid to methane and carbon dioxide. The experimental approach is to construct, from pure cultures, defined mixtures of bacteria so that the food chain, containing the necessary catalysts for the conversion of carbohydrate to methane, may serve as a model to define microbial interactions at the biochemical level. Knowledge of these interactions is pivotal to the design and efficient operation of anaerobic digesters for the production of methane from biomass.

37. THE INSTITUTE OF PAPER CHEMISTRY
Appleton, Wisconsin 54912

RAMAN MICROPROBE INVESTIGATION OF MOLECULAR STRUCTURE AND ORGANIZATION IN THE NATIVE STATE OF WOODY TISSUE — $30,700
Rajai H. Atalla
Chemical Sciences Division

The objectives of this project are to establish, by Raman microprobe spectroscopy, the variability of molecular structure and organization in the cell walls of native woody tissue. More specifically, the objectives are to determine the structures and molecular orientations of celluloses and lignins at different points within individual cell walls. A Raman microprobe system has been assembled and procedures for recording spectra from 1 μm domains, within cell wall sections, have been established. Polarized Raman spectra have been recorded with polarization parallel and perpendicular to planes of the cell walls. They show evidence of molecular orientation relative to the plane of the cell wall for both cellulose and lignin. Spectra have been recorded for both longitudinal and transverse sections in tissues from black spruce (Picea mariana) and from loblolly pine (Pinus taeda L). Variations in composition have been detected within the secondary wall of an individual cell, as well as between adjacent cells in the same annual ring. Future work will be directed at more complete characterization of molecular organization and variability in native tissues, and at interpretation of the spectral features associated with other components of the cell walls. The information developed is important both for fundamental understanding of the structure of the cell walls, and for analysis and design of industrial processes which use biomass as a primary resource.

38. IOWA STATE UNIVERSITY
Ames, Iowa 50011

PROLINE METABOLISM IN PLANTS UNDER ENVIRONMENTAL STRESSES — $56,980 (15 months)
Cecil R. Stewart
Department of Botany

The objective of this project is to understand the subcellular mechanism which causes proline to accumulate under various environmental stresses. One of the known effects which contributes to proline accumulation is the inhibition of proline oxidation, a mitochondrial process. This process has been characterized with respect to energy metabolism and we have shown that proline uptake into mitochondria is protonmotive. The rate of uptake of proline exceeds the rate of oxidation. An inhibitor of proline oxidation has been identified which mimics the effects of stress. This inhibitor will be useful in determining the effects of stress which inhibit proline oxidation. It is likely that the control on proline oxidation is at the level of uptake into the mitochondria. Control of the rate of proline oxidation is a normal metabolic function, not an abnormal effect of stress.

The effects of salt stress on proline metabolism have been determined and compared to those due to drought. It appears that there is a common metabolic mechanism which causes proline to accumulate under both stresses. Additional experiments have been conducted which support the hypothesis that proline accumulates in response to an osmotic imbalance in the cell. Under stress, inorganic ions are accumulated in the vacuole. Proline accumulates in the cytoplasm to serve as a compatible osmoticum, balancing the osmotic potential between the two cellular compartments.

These results contribute to our knowledge of how plants adapt to adverse environmental conditions. This information is useful in improving plant productivity in marginal environments.

39. UNIVERSITY OF KENTUCKY
Lexington, Kentucky 40546

PHYSIOLOGY/BIOCHEMISTRY OF PHOTOACTIVATION OF OXYGEN EVOLUTION; PROBES FOR THE S-STATE PROTEIN — $28,328 (two years)
George M. Cheniae
Agronomy Department

The objectives of this work are: 1) to determine the minimal oxidation/reduction reactions and sequences involved in the photoactivation of the oxygen-evolving "enzyme" of photosynthesis; 2) to identify the protein(s) synthesized on chloroplast 70S ribosomes that are required in the photoactivation of Photosystem II donor as well as O_2 evolution following photoinhibition of Photosystem II; 3) to identify and characterize the thylakoid polypeptides required for photosynthetic O_2 evolution. Mutational analyses, conventional extraction/reconstitution analyses and affinity/photoaffinity probes are employed in efforts to identify the Mn-containing oxygen evolving enzyme of photosynthesis.

40. CHARLES F. KETTERING RESEARCH LABORATORY
Yellow Springs, Ohio 45387

THE BASIS FOR THE COMPETITIVENESS OF RHIZOBIUM JAPONICUM IN THE NODULATION OF SOYBEAN — $77,740
William R. Evans, Wolfgang D. Bauer
Enhancement of Plant Productivity

The long range goal of our studies is to determine which characteristics would enable an inoculated Rhizobium strain to compete effectively against indigenous soil rhizobia in nodulating soybean. At present, Rhizobium inocula contribute little to nodulation of host plants in the field because most field soils contain indigenous populations of rhizobia that out-compete the inoculated rhizobia. Genetic engineering of Rhizobium inoculum strains to improve their nitrogen-fixing potential will thus be of little value unless competitive inoculum strains are developed. Studies in our laboratory established that the susceptibility of soybean root cells to nodulation is transient and developmentally restricted to small regions located just above the growing tips of the roots. We are attempting to determine the physiological and genetic characteristics that would enable an inoculum strain to colonize the infectible regions of the root system more aggressively than indigenous strains and to infect these regions more rapidly and efficiently. Attachment of rhizobia to the root surface is an important aspect of colonization. Strong attachment of rhizobia to roots, i.e. attachment not broken by gentle washing, appears to be mediated by polar pili in several strains examined. In earlier studies various strains of R. japonicum, the soybean symbiont, were found to differ significantly with respect to their efficiency of infection initiation. We are currently assessing the competitive importance of these differences in efficiency by inoculating seedlings in soil or artificial soil with mixtures of an efficient and an inefficient strain. We are developing new computerized methods for determining and analyzing nodule occupancy by particular strains, and also determining the relative advantage enjoyed by indigenous strains over inoculum strains as a consequence of their uniform distribution throughout the soil.

41. LEHIGH UNIVERSITY
Bethlehem, Pennsylvania 18015

A GENETIC APPROACH TO SECRETION AND HYPERPRODUCTION OF CELLULASE BY TRICHODERMA — $68,500

Bland S. Montenecourt and Jeffrey A. Sands
Department of Biology and The Biotechnology Research Center

The objectives of this project are to delineate the genetics of cellulase secretion in T. reesei through the construction of a series of hypercellulolytic mutants and temperature sensitive mutants and to analyze the genetic lesions through the parasexual cycle and protoplast fusion. It is anticipated that an understanding of the series of events between synthesis of a protein and the eventual secretion of that protein will provide useful information upon which to base new selection systems for the isolation of superior hypercellulolytic mutants. We are also looking at the effect of various secretion inhibitors (cytochalasin A, benomyl, 2-deoxyglucose) on cellulase production by Trichoderma and have isolated a number of mutants resistant to these drugs. One new TS mutant has been studied in considerable detail: at 37°C it grows rapidly but does not secrete cellulase; at the permissive temperature, it hyperproduces endoglucanase (350 IU/ml), showing a 2-fold increase in specific activity of this enzyme.

42. MARTIN MARIETTA LABORATORIES
Baltimore, Maryland 21227

STUDIES OF PHOTOSYSTEM II USING ARTIFICIAL DONORS — $85,630

Richard Radmer
Biosciences Department

The objective of this project is to gain an understanding of photosynthetic O_2-evolution, a poorly understood and profoundly important process. Most of these studies make use of competitive inhibitors of H_2O oxidation, such as hydroxylamine, hydrazine, and their derivatives. (These compounds which are all analogs of two molecules of H_2O, in varying degrees share the ability to compete with and override H_2O oxidation without destroying the O_2 system.) By the use of mass spectrometric and fluorescence techniques we monitor the interactions of these compounds under various conditions with the O_2-evolving (H_2O oxidizing) system of isolated spinach chloroplasts. Our results enable us to infer some chemical and structural characteristics of the O_2-evolving site.

43. UNIVERSITY OF MARYLAND
College Park, Maryland 20742

ENERGY-DEPENDENT CALCIUM TRANSPORT MECHANISMS IN PLANT MEMBRANES — $62,836
Heven Sze
Department of Botany

The objectives of this project are (i) to identify and characterize active calcium (Ca) transport systems in plants and (ii) to understand the mechanisms that regulate Ca fluxes. Plant tissues include tobacco tissue callus (Nicotiana tabacum), oat roots (Avena sativa) and corn roots (Zea mays). We are using an in vitro approach developed previously in our laboratory to study Ca transport. Organelles and specific membrane vesicles are isolated and purified by differential and density centrifugation; and 45-Ca uptake is measured by a filtration procedure. At least two types of ATP-dependent Ca transport systems have been identified in microsomal vesicles using specific inhibitors and stimulators: one requires a pH gradient and one does not. These two types of Ca transport systems will be separated and characterized and the membrane identity will be determined. To understand how Ca fluxes are regulated, the effect of phyto-hormones and fungal toxins on the various Ca transport systems will be studied. One promising system is the Helminthosporium maydis T toxin which affects Ca transport into isolated mitochondria in vitro. The effect of toxin on active proton and Ca transport into other subcellular membranes will be determined. The mode of toxin action in decreasing Ca uptake into mitochondria will be examined. Ca levels are important in regulating various physiological and biochemical processes. These studies of active Ca fluxes are central to our understanding of not only the mechanism and regulation of solute transport but also the regulation of plant growth and development.

44. UNIVERSITY OF MASSACHUSETTS
Amherst, Massachusetts 01003

CONVERSION OF CELLULOSE TO ETHANOL BY MESOPHILIC BACTERIA — $77,000 (16 months)
Ercole Canale-Parola
Department of Microbiology

The objectives of this project are i) to obtain from natural environments, or by means of mutagenic techniques, strains of mesophilic bacteria capable of fermenting cellulose with maximum production of ethanol, and ii) to study the metabolic processes responsible for the anaerobic conversion of cellulose to ethanol by these bacteria. The procedures used for the isolation of ethanol producers are designed to select for diverse cellulolytic bacteria and involve culture media of varied composition, inocula from different natural environments, different types of cellulosic materials as growth substrates, and a variety of cultural conditions. The fermentation products and the phenotypic characteristics of the isolated strains are determined. Ethanol production from cellulose is studied under different cultural conditions, in pure cultures and in mixed cultures with Zymomonas mobilis. Studies on the inducibility of the cellulase systems of the isolates by pentoses, hexoses, and disaccharides are carried out. Another experimental approach used is aimed at cloning cellulase system genes from mesophilic cellulolytic bacteria into a suitable vector plasmid and then introducing that plasmid into cells of Z. mobilis. The objective of this part of the research is to obtain Z. mobilis strains capable of fermenting cellulose. The bacterial strains isolated in the course of this research and the information obtained on their metabolism will be useful in the development of efficient industrial processes for the conversion of cellulosic materials to ethanol.

45. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824-1312

CONTROLLED MEDIA FOR PLANT TISSUE CULTURE $55,000
Norman E. Good
Department of Botany and Plant Pathology

The objective of this research is to produce plant tissue culture media which are reasonably stable during the rather long culture periods required. The intent is to develop complexes of the plant hormones which can serve as generous reservoirs which break down at various predictable rates, thus providing a range of steady-state levels. At the same time metabolically inert hydrogen ion buffers with suitable low pKa's are being developed so that the hydrogen ion concentrations of media can be more closely regulated. A large number of indoleacetyl amino acids have been prepared already to serve as auxin sources and these show considerable promise as determinants of diverse callus growth and organogenesis. For instance, indoleacetyl-L-alanine releases free indoleacetic acid relatively quickly and supports massive callus growth, indoleacetyl-L-phenylalanine releases free indoleacetic acid slowly and supports primarily shoot production. Complexes of cytokinins with sugars are also being prepared but have not yet been tested. Intermediates for the synthesis of promising buffers are being assembled.

46. UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55104

PHYSIOLOGY AND GENETICS OF METHANOTROPHIC BACTERIA $70,066
Richard S. Hanson
Gray Freshwater Biological Institute

The objectives of this project are to develop genetic techniques for studying methylotrophic bacteria, to map several genes to biosynthetic and catabolic pathways and to characterize specific and non-specific methane monooxygenases. Three bacteria are employed; Methylobacterium organophilum strain XX, a type II facultative methylotroph; Organism SB1, a type II obligate methylotroph and Methylomonas 761, a type I methylotroph that obligatorily requires methane or methanol as an energy source but its growth rate is increased 10 fold by the addition of glucose or amino acids as carbon sources. Methylomonas 761 is a unique type I methylotroph with a complete glycolytic pathway and Krebs cycle. A conjugative plasmid from Organism SB1 that mobilizes chromosomal markers to Pseudomonas species has proven very useful for the in vivo cloning and mapping of several amino acid markers from this methylotroph. A restriction map of this plasmid is nearly complete. The particulate and soluble methane monooxygenases from this species have very different substrate specificities and are being characterized by comparing their subunit composition and antigenic similarities. A newly constructed plasmid vector containing a cosmid gene, genes for kanamycin and tetracycline resistance, seven unique restriction sites and the replicon and mobilization functions of pRK 290 have proven useful for cloning genes of the methanol operon of M. organophilum strain XX.
We now have tools for studying the genetics of amino acid biosynthesis and one carbon metabolism in three different groups of methylotrophs. We intend to complete a map of genes that code for enzymes and regulatory functions involved in one carbon metabolism, to further investigate the unusual properties of Organism SB1 in order to understand its requirement for one carbon energy sources.

47. UNIVERSITY OF MINNESOTA
St. Paul, Minnesota 55108

CORN STORAGE PROTEIN - A MOLECULAR GENETIC MODEL — $70,000
Joachim Messing
Department of Biochemistry

The objective of this proposal is to study the Zein multigene family in Zea mays. The approach uses a new cDNA cloning procedure to isolate full length zein cDNA clones. Clones of different zein subfamilies are found and the microheterogeneity within and between subfamilies is studied by DNA sequencing. The comparison of cDNA and genomic sequences of the A30 subfamily shows some very interesting results. The Z4 genomic clone is an active gene because it matches with one cDNA clone very closely. There are two size classes of zein proteins within one subfamily which differ by a 32 amino acid residue repeat in the middle of the protein. Two poly-A addition signals appear in the 3' end of the zein messages and both are used. A second subfamily, A20, will be analyzed the same way, and then compared with the A30 subfamily. It will be seen, how the 5' leader sequences and the 3' non-translated region are conserved between the two subfamilies. Differences in the signal sequence, the repeated structure, and the carboxyterminus will be of interest in the understanding of the zein protein structure. Zein proteins determine the protein yield and the nutritional quality of corn, a major crop in our agricultural industry.

48. UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

THE MECHANISM OF SWITCHING FROM AN ACIDOGENIC TO A BUTANOL-ACETONE FERMENTATION BY CLOSTRIDIUM ACETOBUTYLICUM — $73,000
Palmer Rogers
Department of Microbiology, Medical School

The overall goal of the experimental work proposed is to elucidate in molecular terms the regulation of the four-branched fermentation pathway in Clostridium acetobutylicum. The roles and interactions of the regulating devices in the overall physiologic program of this obligate anaerobe will be investigated.

The experiments are designed to provide knowledge of how the switching of the fermentation between the acidogenic and solventogenic phases is related to H_2 and NAD(P)H on the one hand or to the sporulation program on the other. The specific modes of regulation and allosteric modulators for the enzymes in the four branches leading to butanol, acetone, butyrate and acetate will be determined. A selection system for isolating acid-less mutants in anaerobic plate culture will be developed and mutants that are asporogenous will be isolated. The mutants will be used to develop a genetic system in Clostridium acetobutylicum based on protoplast fusion.

It is hoped that the fundamental knowledge gained will provide a clearer picture of the normal regulation circuitry of this important anaerobe so that a scientific basis is established for future genetic programming of the solventogenic fermentation.

49. UNIVERSITY OF MINNESOTA
St. Paul, Minnesota 55108

FEASIBILITY OF MOLECULAR HYBRIDIZATION TECHNIQUES IN STUDYING GENOMIC ORGANIZATION — $60,055

Irwin Rubenstein, Department of Genetics & Cell Biology
Ronald L. Phillips, Department of Agronomy and Plant Genetics

We propose to develop physical methods to determine the chromosomal location of isolated genomic segments. The first procedure will use a modified dot hybridization technique combined with the use of DNAs from a series of trisomic, disomic and monosomic maize plants. We will attempt to demonstrate the capability to distinguish an expected 2:1:3 hybridization ratio versus a 1:1:1 ratio depending on whether or not a particular sequence is in that chromosome. The second procedure to be developed is that of *in situ* hybridization using immunofluorescent antibodies or 125I-Labeled probes to detect sequences present at low reiteration frequencies. Our objective will be to develop a reasonably rapid technique to determine the chromosomal location of unique sequences. We hope that these approaches will allow us to map any gene sequence cloned by recombinant DNA techniques.

50. UNIVERSITY OF MISSOURI
Columbia, Missouri 65211

PHOTOSYNTHESIS AND CLONING IN CYANOBACTERIA--A SYSTEM FOR THE BIOCONVERSION OF SOLAR ENERGY — $72,129

Louis A. Sherman
Division of Biological Sciences

The objective of this study is to identify and clone genes coding for photosynthetic membrane proteins in the cyanobacterium, *Anacystis nidulans* R2. This strain can be transformed with exogenous DNA and it possesses indigenous plasmids. We have constructed hybrid cloning vectors that can replicate in both *A. nidulans* and *Escherichia coli* and that can confer ampicillin and chloramphenicol resistance to both organisms. We have cloned the rRNA operon from *A. nidulans* onto one vector (pSG111) and shown that the recombinant plasmid can be stably maintained extrachromosomally. We have also isolated temperature-sensitive photosynthesis mutants and herbicide-resistant mutants of *A. nidulans*. We are now using two approaches for the identification and cloning of specific photosynthesis genes. We have produced a library of *A. nidulans* chromosomal DNA in the vector pSG111. By transforming this library into specific mutants, we can identify genes by complementation. This has successfully been accomplished in at least two cases. We are also using heterologous probes from chloroplast and *E. coli* DNA to identify photosynthesis genes. This procedure has enabled us to clone the *A. nidulans* genes coding for the large and small subunits of RuBP carboxylase, three subunits of the ATPase complex, a membrane-bound hydrogenase, and a Ca^{+2}-binding protein homologous to calmodulin. Additionally, we have found that sequences homologous to these probes are located on plasmid as well as chromosomal DNA. Most of these plasmid-encoded genes are on the 33 Mdal plasmid; however, we have detected the presence of a very large plasmid (>120 Mdal) that also encodes photosynthesis genes. The gene coding for the chloroplast 32kDa herbicide-binding protein hybridizes to three chromosomal and two plasmid sequences. The three chromosomal genes are also present in two DCMU-resistant mutants; despite the presence of multiple genes, wild-type cells can be readily transformed with the DCMU resistance trait.

51. MOUNT SINAI SCHOOL OF MEDICINE OF THE CITY
UNIVERSITY OF NEW YORK
New York, New York 10029

THE RESPIRATORY CHAIN OF ALKALOPHILIC BACTERIA — $78,020
Terry Ann Krulwich
Department of Biochemistry

Obligately alkalophilic bacteria contain extraordinarily high concentrations of membrane-bound respiratory chain components and an apparently complex respiratory chain, with many carriers that are distinguishable on the basis of their midpoint potentials. It has been proposed that the alkalophile respiratory chain possesses structural/functional properties, of which the complexity is a part, which facilitate particularly effective energy transduction at high pH. Initial studies of H^+ translocation during respiration by whole cells of alkalophilic Bacillus firmus RAB support this hypothesis. Further studies of H^+ pumping will be conducted using whole cells and reconstituted systems. The latter will first involve a study of cytochrome oxidase purified from B. firmus RAB. This respiratory chain complex has been purified to homogeneity. It will now be characterized and studied in proteoliposomes.

52. NATIONAL INSTITUTE OF GENERAL MEDICAL SCIENCES
National Institutes of Health
Bethesda, Maryland 20205

GENBANK (TM), THE GENETIC SEQUENCE DATA BANK — $40,000
Christine Carrico

GenBank (TM), the Genetic Sequence Data Bank, is an internationally available repository of all reported nucleotide sequences greater than fifty nucleotides in length, annotated for sites of biological interest and checked for accuracy. As of June 1, 1983, GenBank contained 1.70 million bases, comprising 2082 sequences. The data bank is operated under contract to Bolt Beranek and Newman Inc. (BBN) of Cambridge, MA. Data collection, verification, entry and annotation is performed under the direction of Dr. Walter Goad at Los Alamos National Laboratory, while distribution, user support services and overall data bank management are performed by BBN. This resource, co-sponsored by the National Institute of General Medical Sciences, National Cancer Institute, National Institute of Allergy and Infectious Diseases, and Division of Research Resources, all of NIH, and the Department of Energy and the National Science Foundation, is of particular interest to geneticists and molecular biologists. A copy of the database is available for a modest fee on computer-readable magnetic tape to anyone requesting it. Dial-up on-line access is also available to anyone, but only a limited number of users can be accommodated at any one time. The first yearly hard copy edition of the database will be available in early 1984.

53. UNIVERSITY OF NEBRASKA-LINCOLN
Lincoln, Nebraska 68583-0718

BIOCHEMICAL AND PHYSIOLOGICAL CHARACTERIZATION OF HIGHER PLANTS WITH REDUCED PHOTORESPIRATION — $53,949
Raymond Chollet
Department of Agricultural Biochemistry

This project is designed to further our understanding of mechanisms which may reduce photorespiration in higher plants. Leaf anatomical/ultrastructural features and CO_2 exchange characteristics of the crucifer Moricandia arvensis are intermediate between those of C_3 and C_4 plants and show similarities to the C_3-C_4 intermediate species, Panicum milioides. In comparison to C_3 plants, both species exhibit reduced rates of photorespiration [Holaday et al. (1982) Plant Sci. Lett. 27, 181-189]. Low in vitro activities of certain key C_4-related enzymes suggest that a limited C_4-like CO_2 concentrating mechanism is not responsible for reducing photorespiration in either M. arvensis or P. milioides [Holaday et al. (1981) Biochim. Biophys. Acta 637, 334-341 and unpublished data]. Pulse-chase $^{14}CO_2$ incorporation experiments with these intermediate species indicate that the pathway for carbon assimilation is similar to that in the C_3 plants, M. foetida and Glycine max [Holaday & Chollet (1983) Plant Physiol. in press]. There is NO evidence of C_4 photosynthesis. After a 6-s exposure to air containing 310 µl $^{14}CO_2$/L, only about 6% of the total ^{14}C fixed is present in malate and aspartate in both M. arvensis and P. milioides. During subsequent chase periods in $^{12}CO_2$-air there is little apparent turnover of these C_4 acids. However, there are notable differences among the species examined in the labelling of glycine: with M. arvensis after 36 s, 20% of the ^{14}C is found in this key photorespiratory metabolite compared to 15% with M. foetida, 14% with P. milioides and 9% with G. max. Additionally, following a similar chase period at subatmospheric levels of CO_2 (100 µl/L), the percentage of ^{14}C in glycine increases 2- to 3-fold in P. milioides and the C_3 plants, but only 0.2-fold in M. arvensis. These apparent differences in glycine metabolism may relate to the mechanism by which photorespiration is reduced in M. arvensis. Future investigations will focus on photorespiratory glycine and glycolate metabolism in this intermediate species.

54. UNIVERSITY OF NEBRASKA
Lincoln, Nebraska 68583-0722

VIRUSES OF EUKARYOTIC GREEN ALGAE — $62,000
James L. Van Etten
Department of Plant Pathology

We have recently isolated and partially characterized four distinct dsDNA viruses which replicate in Chlorella-like green algae symbiotic with Hydra and Paramecium. One of these viruses, PBCV-1, also synchronously infects and replicates in two culturable Chlorella. This has allowed, for the first time, the production of mg quantities of a eukaryotic algal virus as well as the development of a plaque assay for PBCV-1. The PBCV-1 Chlorella system is the first example of a virus infecting any eukaryotic plant which can utilize procedures directly adapted from those used to study bacteriophage.

The objective of this proposal is to determine the structural organization and properties of the large viral genome (ca. 280 kbp) and the nature and function of the viral gene products. The research has several potentially important long range implications. Studies on PBCV-1 will: (i) provide an opportunity to study a new type of virus-host relationship, (ii) determine the role it plays in symbiosis, (iii) demonstrate the usefulness of PBCV-1 or PBCV-1 DNA as a vector for transferring genes into other algae or higher plants, and (iv) determine if PBCV-1 or PBCV-1 lysates contain a new source of plant cell wall degrading enzymes. Finally studies on the regulation and expression of the dsDNA viral genome in the host will provide new information on gene regulation in eukaryotic plants.

55. NEW YORK STATE DEPARTMENT OF HEALTH
Center for Laboratories and Research
Albany, New York 12201

METHANE PRODUCING BACTERIA: IMMUNOLOGICAL CHARACTERIZATION — $47,000
Conway de Macario, E.,* Macario, A.J.L.,* and Wolin, M.J.°
*Laboratory of Immunology
°Laboratory of Environmental Biology and Field Services

The objective of this project is to use immunologic methods for identification and classification of methane-producing bacteria (methanogens). A comprehensive panel of calibrated antibody probes is derived from rabbit antisera. These probes are used to elucidate the antigenic fingerprint of reference methanogens. A standard chart of antigenic fingerprints is generated and is utilized as a reference to classify new strains on the basis of their own fingerprints. Isolates from a variety of ecologic niches in this country and abroad are fingerprinted. The data are examined together with other immunologic results (e.g. cross-adsorption and serial dilution) and studied considering information obtained in other laboratories, such as nucleic acid homologies, physiologic characteristics, and cell-wall chemistry to establish the phylogenetic position of the new isolate. Immunochemical dissection of taxonomically important surface molecules (antigenic determinants) is carried out with antibody probes by means of inhibition-blocking experiments and direct binding assays. These studies are being applied to identification and enumeration of methanogenic bacteria in practically important methane producing systems, i.e. systems for production of natural gas from biomass, waste decomposition systems and natural ecosystems where methane production is an important component of the carbon cycle. The antigenic fingerprints have demonstrated that several methanogens that have been isolated recently belong to new taxonomic groups and are distinctly different from all other previously characterized methanogens. Immunochemical dissection has also helped to identify several antigenic cell surface components of methanogens.

56. STATE UNIVERSITY OF NEW YORK AT BINGHAMTON
Binghamton, New York 13901

GENE-ENZYME RELATIONSHIPS IN SOMATIC-CELLS AND THEIR ORGANISMAL DERIVATIVES IN HIGHER PLANTS — $90,000
Roy A. Jensen
Center for Somatic-cell Genetics & Biochemistry

Comprehensive and systematic approaches will be taken to isolate regulatory mutants which excrete tyrosine, phenylalanine or tryptophan in cultured cells of tobacco (Nicotiana silvestris). Mutants will be isolated by selecting for resistance to various antimetabolite analogs of aromatic amino acids in initially haploid cell populations. Resistant mutants will be sought whose phenotype of analog resistance is temperature-sensitive, genetically stable, and which will regenerate (at least at low temperature). Mutants will be screened for pathway deregulation by scoring the ability of candidate callus fragments to cross-feed appropriate Bacillus subtilis auxotrophs. Clonal purity of mutants will be rigorously established through several rounds of protoplast plating. Biochemical and enzymological characterization of key aromatic pathway enzymes of wild type will be completed to allow the acquisition of a collection of genetic markers that are rigorously defined biochemically. Isolation strategies are proposed based upon the current enzymological data available, the in vitro and in vivo effects known for some analogs, and upon the availability of an in vivo inhibitor of phenylalanine-ammonia lyase activity. The expression of particular mutations at the cell-culture level will be compared with the impact of the same mutations at the organismal level whenever possible. Dominance relationships can be assessed following formation of somatic-cell hybrids through protoplast fusion. The gene dose relationships of regulatory mutations with ploidy state will be examined by comparing specific activities of appropriate enzymes and through measurement of excretion rates of aromatic amino acids. The detailed study of pathway arrangement and regulation in wild type in comparison with deregulated mutants will contribute heavily to an overall appreciation of a metabolic pathway which is the focal point of a very large fraction of higher plant metabolism.

57. UNIVERSITY OF NORTH CAROLINA
Chapel Hill, NC 27514

THE ISOLATION AND CHARACTERIZATION OF β-GLUCOSIDASE GENE AND β-GLUCOSIDASE OF TRICHODERMA VIRIDE — $85,000

Darrel W. Stafford
Department of Biology

mRNAs have been isolated from Trichoderma reesei QM9414 cultures grown in the presence of cellulose for varying times. Electrophoretic analysis of in vitro translation products which had been precipitated with antibody to cellobiohydrolase I (CBH) I) indicated high levels of CBH I mRNA at 20hr, 42hr, and 72hr post-induction. No translational product was precipitated by CBH I antibody from translation incubations using mRNA isolated from cultures induced for 7 days. A β-glucosidase immunoprecipitable translation product was detectable only at 20hr post-induction.

The amino terminal portion of CBH I has been published by Pettersson. A mixture of oligonucleotides designed to be specific for amino acids 16-19 of CBH I was synthesized, 5'-labeled with ^{32}P and used to prime the synthesis of cDNA by reverse transcription of mRNA from 20hr induced cultures. The resulting reverse transcript of single strand DNA was fractionated by acrylamide electrophoresis and the DNA was sequenced by the Maxam and Gilbert technique. The sequence (when translated into protein sequence) agreed perfectly with the amino acid terminal sequence published by Pettersson. Genomic and cDNA clones for CBH I were identified using this authentic CBH I cDNA as an hybridization probe. The genomic and cDNA clones of CBH I are being sequenced.

We have also synthesized oligonucleotides for probes for CBH II and endo-glucanase II and have selected, in a first screen, phage which hybridize to the probe designed to be specific for CBH II.

58. OHIO STATE UNIVERSITY
Columbus, Ohio 43210

DEVELOPMENT OF GENETIC SYSTEMS FOR ANALYSIS OF THE OBLIGATE ANAEROBE METHANOBACTERIUM RUMINATIUM FS — $63,196

John N. Reeve and James I. Frea
Department of Microbiology

The goal of this project is to develop techniques which will facilitate genetic analyses of methane producing micro-organisms. We are isolating antibiotic resistant mutants to provide selective genetic traits. DNA prepared from antibiotic resistant strains is being used to determine if methanogens can be transformed by direct exposure to DNA or following conversion of methanogens to protoplasts. The size and structure of the DNA of several Methanococcus species is being characterized by use of restriction enzymes and two dimensional agarose gel electrophoresis. Several genes have been cloned by in vitro recombinant DNA procedures from Methanobrevibacter smithii, Methanosarcina barkeri, and Methanococcus vannielli which are functionally expressed in Escherichia coli as demonstrated by complementation of auxotrophic mutations of Escherichia coli. The fine structure of these genes is being determined for comparison with the known structure of the analogous genes already characterized from bacteria. Availability of specific cloned methanogen genes has led to the instigation of a search for mutations in these genes in the methanogenic species from which the genes were originally isolated. Ultraviolet light and mitomycinC are being used as mutagens. If such mutants can be isolated then they will be exposed to preparations of DNA containing the cloned genes, as donor DNA, in procedures designed to develop genetic transformation systems. Analyses of cloned methanogen DNAs show that there are several repetitive sequences in the genomes of methanogens. Current studies are aimed at determining if these sequences show the characteristics of transposable elements and if they can be modified by in vitro enzymatic procedures to act as vectors for introduction and integration of DNA into the genomes of methanogens.

59. UNIVERSITY OF OKLAHOMA
Norman, Oklahoma 73019

METABOLISM OF FATTY ACIDS BY SYNTROPHOMONAS WOLFEI — $36,231
Michael McInerney
Department of Botany and Microbiology

The objective of this project is to study the metabolism of fatty acids by the anaerobic hydrogen-producing fatty-degrading bacterium, Syntrophomonas wolfei. The degradation of fatty acids is often the rate-limiting steps in the conversion of organic matter to methane and carbon dioxide. However, little is known about the metabolism of the bacteria responsible for these reactions because they have very slow growth rates and can only be grown in co-culture with hydrogen-using bacteria. Methods to grow S. wolfei in pure culture by gas recycling after hydrogen removal will be developed as well as techniques for mass-culturing S. wolfei in pure culture or in co-culture. Methods will also be developed to obtain cell-free extracts of S. wolfei free from contamination by cells of the hydrogen user by selective lysis of S. wolfei cells with lysozyme. These methods will be used to determine the pathways for fatty and degradation, hydrogen production and poly-β-hydroybutyrate formation in S. wolfei. The implications of this research are of primary importance to the optimization of any commercial process involving anaerobic microorganisms for fuel gas production or waste treatment.

60. UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

FACTORS GOVERNING LIGHT DRIVEN ELECTRON AND PROTON TRANSLOCATION IN PROTEINS ACROSS MEMBRANES — $80,000
F. Leslie Dutton
Department of Biochemistry & Biophysics

The goal of this project is to reveal the properties of the individual steps that lead to electrogenic charge separation and recombination across membrane proteins. The photochemical reaction center from Rhodopseudomonas sphaeroides, cytochrome c and quinones represent the principal system used. The means to the goal of this project is to achieve a closer experimental access to the electrical properties of the electrogenic reactions. This will be done by organizing the proteins in the form of planar bilayers or in the form of protein mono- and multilayers deposited on planar substrates and electrode material. Use of flash activation and kinetic analysis (in several cases down to helium temperatures), use of systematic biochemical alteration of the ΔG of key reactions, and use of the effects of applied potentials should provide information on the biochemical nature of the electrogenic events and provide much needed experimental contributions that will be useful to understanding the factors that govern electron and proton translocation.

61. PURDUE UNIVERSITY, Dept. of Horticulture
West Lafayette, Indiana[1]
NATIVE PLANTS INC.; Salt Lake City, Utah[2]

REGULATION OF PROTEIN AND mRNA METABOLISM IN SALT TOLERANT AND INTOLERANT CULTURED HIGHER PLANT CELLS — $80,000

R.A. Bressan[1], A.K. Handa[1], P.M. Hasegawa[1], T.H. Ulrich[2], G.J. King[2], T. Melantjaris[2]

The proposed work has the following objectives: 1) to identify specific gene products (protein and mRNA molecules) which are associated with salt shock and eventual tolerance in cultured plant cells 2) determine if such proteins and mRNAs are the same as those elicited by other stresses, e.g. heat shock 3) determine if such proteins and mRNAs are the same as those associated with PEG-induced water stress tolerance in tobacco and other plant species 4) determine whether abacisic acid can affect the salt tolerance of cultured cells and whether it can induce changes in protein and mRNA synthesis which are associated with tolerance and measure the changes in ABA levels in cells as they undergo adaptation and become tolerant 5) determine to what extent salt shock and/or tolerance specific proteins are associated with cell membrane fractions and organelles 6) determine how the synthesis of salt shock and tolerance specific mRNAs and proteins is regulated e.g. all at transcription, in a coordinated fashion, etc. 7) determine the genomic organization of salt shock and tolerance genes, e.g. their relative chromosomal locations, level of amplification, if any, and regulatory and sequence similarities.

62. PURDUE UNIVERSITY
West Lafayette, Indiana 47907

STUDIES ON THE STRUCTURE AND EXPRESSION OF GENES IN HIGHER PLANTS — $120,000

Brian A. Larkins and Donald E. Foard
Department of Botany and Plant Pathology

The objective of this project is to isolate and characterize the genes encoding the low molecular weight protease inhibitors from soybean (Glycine max L. Merr). This group of proteins includes the Bowman-Birk protease inhibitor and its related family of isoinhibitors, PI I-IV. Characterization of these polypeptides reveals that they are rich in sulfur-containing amino acids and that their amino acid sequences are highly conserved. A major aspect of the research is to prepare a cDNA probe for the BBI by synthesizing complementary DNA from messenger RNA. This cloned probe is used to isolate the corresponding gene from a soybean genomic library. Information which has been obtained reveals that the Bowman-Birk inhibitor is encoded by a single gene in the soybean genome which is under developmental regulation. Nucleotide sequence analysis of this gene reveals that it contains no intervening sequences. The results obtained from this research will be useful in gene transfer experiments designed to improve the nutritional value of seeds and increase the natural plant protection by engineering multiple copies of the BBI gene in soybean.

63. THE ROCKEFELLER UNIVERSITY
New York, N.Y. 10021

EXPRESSION OF NUCLEAR GENES ENCODING THE SMALL SUBUNIT OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE. $85,000
Anthony R. Cashmore
Laboratory of Cell Biology

The aim of this proposal is to characterize the nuclear genes from pea encoding the small subunit of ribulose-1,5-bisphosphate carboxylase. Two of these genes have been isolated and sequenced. In collaboration with Luis Herrera-Estrella and Marc Van Montagu in Gent, Belgium, we have examined the expression of these genes in tobacco cells after transfer with Agrobacterium. A 900 nucleotide 5' non-coding fragment from the small subunit gene was linked to the coding region of the bacterial gene chloramphenicol acetyltransferase. Expression of this hybrid gene was observed in tobacco cells, and furthermore the expression was dependent on, and inducible by light. One aspect of future work will involve in vitro mutagenesis studies aimed at defining the DNA sequence requirements necessary for this light induction.

64. RUTGERS - THE STATE UNIVERSITY OF NEW JERSEY
New Brunswick, New Jersey 08903

CELLULASE - A KEY ENZYME IN FERMENTATION $52,347
Douglas E. Eveleigh
Department of Biochemistry & Microbiology
Cook College

The objective of this project is to enhance the production of cellulase by the fungus Trichoderma reesei through removal of factors regulating the secretion of the enzyme. The study involves clarification of the discrete stages in the secretory mechanism, and encompasses a study of the T. reesei physiology (Rutgers Medical School), of secretory mutants (Lehigh University) and of cellulase methodology (Cook College). Hypersecreting mutants have been isolated and one class of them shown to possess enhanced amounts of endo-plasmic reticulum. Our immediate results at Cook have shown improved methods of purification of the several components of cellulase, and of identification of the products via high precision liquid chromatography (HPLC).

65. UMDNJ-RUTGERS MEDICAL SCHOOL, Piscataway, NJ 08854 and LEHIGH UNIVERSITY, Bethlehem, PA 18015 and COOK COLLEGE, New Brunswick, NJ 08903

BIOMASS UTILIZATION: BASIC SECRETORY PHENOMENA AND THE CONSTRUCTION OF HYPERCELLULOLYTIC MUTANT OF TRICHODERMA REESEI — $119,894 (FY 82 funds)

B. K. Ghosh & A. Ghosh, Dept. Physiology & Biophysics UMDNJ, Rutgers Medical School; and B.S. Montenecourt & C.I. Sheir-Neiss, Biotechnology Research Center, Lehigh University. Douglas E. Eveleigh, Cook College

Cellulases are important industrial enzymes having potential application in the recycle and use of renewable biomass. Little is known in fungi about their site of synthesis, co- or post-translational modification (e.g., glycosylation, selective proteolysis, etc) and the transport from the site of synthesis to the cell exterior. The objective of this project is to study the phenomena of secretion of the cellulase enzyme complex in Trichoderma reesei wild type (QM6a) and a hypercellulolytic mutant (Rut-C30). Rut-C30 compared to QM6a exhibits: (i) 3-5 fold increase in the yield of cellulase; (ii) enhanced secretion of the cellulase; (iii) proliferation of the endoplasmic reticulum during the logarithmic phase of growth and (iv) resistance to repression of cellulase biosynthesis by glycerol. The specific time sequence of secretion has been pinpointed. Synthesis and secretion of endoglucanase and cellobiase terminate at the end of the logarithmic phase of growth. In contrast, synthesis and secretion of the filter paper activity continue throughout stationary phase. Concomitant releases of other intracellular marker enzymes do not occur suggesting lack of cell lysis. Thus, cellulase secretion is not the result of autolysis. Preliminary cytochemical observations suggest that the endoglucanases may be located in vesicles near the plasma membrane prior to secretion. This will be precisely determined by immunocytochemical methods. Gel electrophoresis (SDS) patterns indicate that the enzymes of the mutant are slightly larger than those of QM6a. Isoelectric focusing of the enzymes shows a greater charge heterogeneity for the endoglucanases of Rut-C30 than QM6a. The Rut-C30 enzymes during the time course of fermentation do not show as much microheterogeneity as the batch culture enzymes. Cause of this microheterogeneity (i.e. glycosylation, proteolysis, etc.) is under investigation.

66. SMITHSONIAN INSTITUTION Washington, D.C. 20560

A PRIMARY LIGHT HARVESTING SYSTEM: PHYCOBILISOMES AND ASSOCIATED MEMBRANES — $60,342

Elisabeth Gantt
Radiation Biology Laboratory
Rockville, MD 20852

Absorption of light for photosynthesis is greatly enhanced in red and blue-green algae by the accessory pigments in the phycobilisome antennae. A large part of the energy absorbed is transferred directly to the reaction centers in the photosynthetic membranes. The structural diversity between the green plants and red and blue-green algae is becoming more apparent. In phycobilisome-containing plants the two photosystems appear to be integrated and not sequestered in separate regions of the thylakoids as in green plants. A spatially integrated system allows for potentially better energy utilization which would be especially important under light limiting conditions. We are using the apparently simpler photosynthetic membranes of the red alga Porphyridium cruentum to determine the topological relationship of the photosystems (I and II), and their relationship with the phycobilisomes. A combination of approaches, involving non-ionic detergent fractionation, antibody production against purified polypeptides of phycobilisome anchor protein(s), and chlorophyll-binding proteins of photosystems I and II, is being applied. Directly related with this are our investigations on photosynthetically active photosystem II-phycobilisome particle preparations which appear to be virtually free of photosystem I. By comparing the composition of the PSII-particles we expect to identify the functional components of the polypeptides catalizing the photosystem II reactions. These investigations are expected to contribute to our understanding of the photo-oxidation of water in oxygen evolving plants.

67. SOUTHERN ILLINOIS UNIVERSITY
Carbondale, Illinois 62901

REGULATION OF ALCOHOL FERMENTATION BY ESCHERICHIA COLI. $60,000
David P. Clark
Department of Microbiology

Our objective is to identify the genes involved in the production of ethanol by the facultative anaerobe Escherichia coli and to elucidate their regulation. Strains in which the two enzyme activities acetaldehyde:CoA dehydrogenase and alcohol dehydrogenase are expressed constitutively in high levels have been used as the starting point for the isolation of mutants lacking these enzymes or with thermolabile enzymes. Mutants lacking only one enzyme are much less frequent than those lacking both activities, suggesting some functional interaction between these two enzymes. This possibility is being investigated by two different approaches. First, the adh operon is being cloned, in order to characterize the various adh genes and their products more closely. Secondly, the two enzymes are being purified, both by classical methods and also by dye ligand chromatography using Cibacron Blue and Procion Red which specifically bind enzymes using NAD as cofactor. The regulation of gene expression is being approached, not only by the use of gene cloning, but also by the isolation of operon fusions in which the regulatory sequences for the adh operon are fused to the β-galactosidase structural gene. Such fusions confirm the anaerobic control of the adh operon and will also allow the isolation of novel regulatory mutants. Understanding the operation and genetic regulation of alcohol fermentation at the molecular level should allow the optimization of alcohol production by fermentation.

68. STANFORD UNIVERSITY
Stanford, California 94305

CLONING AND MAPPING OF EARLY SYMBIOTIC GENES OF RHIZOBIUM MELILOTI $76,630
Sharon R. Long
Department of Biological Sciences

Our research concerns the genes used by Rhizobium meliloti to form nitrogen fixing root nodules on its symbiotic host, alfalfa. We have identified a region which is required for early stages of nodule formation; we have obtained clones representing the DNA of this region and have generated five mutants with lesions in the DNA fragments where the nodulation genes appear to be located. In the coming year, we will generate a fine structure map of that area, by placing transposon insertions at frequent intervals in the locus and by DNA sequencing. We will mutagenize adjacent fragments of DNA also, in order to determine whether any nodulation genes are present there. In addition, we will attempt to clone and map other genes involved in rhizobial infection; we will use the direct-complementation strategy which we have developed for obtaining cloned nodulation genes. This procedure will be carried out on five other nodulation mutants, which appear to be defective in genes other than those already identified and studied by us. The relationship of infection genes to host range genes is another topic which we are interested in. We are beginning a series of experiments designed to clone directly the bacterial genes responsible for host-plant choice. The identification of such genes will be an essential prerequisite for studying their effect on the symbiosis and for manipulating the symbiosis for greater agronomic usefulness.

69. STANFORD UNIVERSITY
Stanford, California 94305

CARBON DIOXIDE AND THE STOMATAL CONTROL OF WATER BALANCE AND PHOTOSYNTHESIS IN HIGHER PLANTS — $44,000

Eduardo Zeiger
Department of Biological Sciences

Stomata provide higher plants with a primary means to adjust to their continuously changing environment. Stomatal control of gas exchange also has a major impact on photosynthetic rates and the water balance of the vegetation.
CO_2 is an important factor affecting mesophyll photosynthesis and stomatal conductance yet its mode of action on stomata remains unknown. Stomata open in low CO_2 concentrations and close in high CO_2, both in light and darkness. The light response is of special interest because of its possible role as a coupling factor between the photosynthetic and stomatal responses of the leaf.
The modulation of light-dependent stomatal responses by CO_2 has been classically assumed to be mediated by guard cell chloroplasts but their recently reported lack of RuBP carboxylase is inconsistent with that hypothesis. However, using fluorescence spectroscopy techniques on guard cell chloroplasts, we found that fluorescence transients associated with photophosphorylation are specifically inhibited by CO_2. These data indicate that, through a yet to be characterized metabolic pathway, CO_2 could modulate the supply of energy for stomatal movements by controlling photophosphorylation rates in guard cell chloroplasts. A role of these organelles in stomatal responses to CO_2 is further indicated by gas exchange studies of the orchid Paphiopedilum, having achlorophyllous stomata, in comparison with its normal relative, Phragmipedium. The CO_2 sensitivity of Paphiopedilum stomata was markedly reduced in the light. These findings are providing us with new research tools to investigate the role of CO_2 in stomatal function. Further progress on these questions should increase our ability to evaluate the impact of CO_2 on plant productivity and the possible consequences of atmospheric CO_2 enrichment on the biosphere.

70. UTAH STATE UNIVERSITY
Logan, Utah 84322

BIOENERGETICS OF THE METHANOGENIC BACTERIA — $81,310

J. R. Lancaster, Jr.
Department of Chemistry and Biochemistry

The objectives of this project are to (1) determine the biochemical components involved in methanogenesis and delineate their functional relationships to each other, and (2) determine the mechanism(s) whereby methane formation results in energy production (ATP synthesis) by the cell. Our approaches involve the application of modern biophysical and biochemical techniques for the measurement of electron transport- and transmembrane ion gradient-linked bioenergetic phenomena. Our initial studies focus on membrane-associated enzymatic activities, including hydrogenase and ATPase. Since the sole function of methane formation by these unique organisms is the production of cellular energy such a perspective should provide a fruitful experimental approach toward the delineation of methanogenic processes in general.

71. WASHINGTON UNIVERSITY
St. Louis, Missouri 63130

GENETIC ENGINEERING WITH A GENE ENCODING A SOYBEAN STORAGE PROTEIN — $63,000

Roger N. Beachy
Department of Biology, Box 1137

The objectives of our studies are to understand the mechanisms that control the expressions of genes encoding the β-conglycinin seed storage proteins of soybeans. Part of that study involves transferring one or more of the storage protein genes to a new plant species and subsequently determining if the gene is expressed, and following the fate of the gene product. During the past year a gene encoding the α'-subunit of β-conglycinin was characterized by DNA sequence analysis. Since the expression of other eucaryotic genes transcribed by RNA polymerase II is controlled by DNA sequences in front of (5') of the gene, we generated a number of DNA fragments that contained the structural gene and varying amounts of DNA 5' of the gene. The amount of DNA varied from (+) 9,000 nucleotides to (-) 14 nucleotides. Each of these DNA fragments (eight in total) are being transferred via a six-step conjugation and transformation sequence, into the Ti-plasmid of Agrobacterium tumefaciens. These bacteria will be used to transform tobacco cells. The Ti-plasmid chosen for this work has been mutated to permit the regeneration of intact, fertile plants from transformed cells. Subsequent experiments will determine if the engineered gene is expressed and whether it is developmentally regulated. We will also determine the fate of the RNA and protein products of the expressed gene. Concurrent with these experiments the gene, under control of a constitutive promoter, will be transferred petunia cells and its expression will be monitored in a similar manner.

72. WASHINGTON UNIVERSITY
St. Louis, Missouri 63130

DEVELOPMENT OF A TUMOR-INDUCING (TI) PLASMID VECTOR FOR PLANT GENETIC ENGINEERING — $70,000

Mary-Dell Chilton
Department of Biology

The Agrobacterium Ti plasmid is a natural gene vector that inserts T-DNA, a specific sector of the plasmid, into host plant nuclear DNA causing tumorous growth. Tumor cells can be genetically engineered by introducing foreign DNA into T-DNA, which then carries it into the host plant. An important problem with this gene vector system is that tumor cells do not regenerate into plants as can normal plant cells. We have constructed a MICRO-Ti plasmid that solves this problem. It is a relatively small plasmid carrying the left and right borders of T-DNA but lacking all of the interior (tumor-inducing) genes of T-DNA save one, the innocuous nopaline synthase gene. MICRO-Ti plasmid has a unique cloning site within T-DNA where foreign genes of choice can be inserted. It is clear that MICRO-Ti can transfer its T-DNA to plant cells when helped by a large plasmid carrying VIR (virulence) genes: although we see no tumorous outgrowth, the plant cells at the site of inoculation synthesize nopaline, a sign that they possess the nopaline synthase gene. It appears that MICRO-Ti can thus be complemented in trans by a VIR helper plasmid. This small vector plasmid, with several refinements, will provide the basis for a convenient and useful genetic engineering vector for crop plants.

73. WASHINGTON STATE UNIVERSITY
Pullman, Washington 99164

REGULATION OF TERPENE METABOLISM — $66,918
Rodney Croteau
Institute of Biological Chemistry, 6340

The volatile plant oils (essential oils) and plant derived resins are finding increasing use as replacements for petroleum based industrial feedstocks, and the potential for the large scale production and expanded use of these renewable resources is considerable. To realize this potential, fundamental knowledge of the biochemistry of essential oil and resin terpenes is needed, particularly as it applies to the regulation of terpene metabolism. This research project is intended to provide an understanding of such regulatory mechanisms at the enzyme level. This objective is being accomplished through the intensive investigation of two model systems (camphor metabolism in Salvia officinalis and menthone metabolism in Mentha piperita) which allows us to probe the control of both biosynthetic and catabolic processes involved in monoterpene accumulation. The pathways of biosynthesis of both monoterpene ketones are being established, as are the sequences of reactions involved in the conversion of both compounds to their water-soluble derivatives which are transported out of the oil gland sites of synthesis to the roots. The enzymes of these pathways are under study. A major focus of the research is the possible hormonal mediation of developmental enzyme level changes (biosynthetic activity decreases as the leaf reaches full expansion) and the possible inductive processes mediated by the terpenes themselves (catabolic activity may be initiated by collapse of the mature oil glands with the monoterpenes "flooding" the surrounding epidermis and adjacent mesophyll tissue). These lines of investigation are being pursued, as is the ultimate fate of the terpene conjugates on transport to the roots. The new information gained from this research will have important consequences for the yield and composition of terpenoid oils and resins that can be made available for exploitation as renewable sources of chemical feedstocks.

74. WASHINGTON STATE UNIVERSITY
Pullman, Washington 99164

DNA TRANSFORMATION OF PLANT CELLS DEFECTIVE IN NITRATE REDUCTASE ENZYME ACTIVITY — $45,144
Andris Kleinhofs and Paul F. Lurquin
Department of Agronomy and Soils and Program in Genetics and Cell Biology

The objective of this research is to develop procedures for plant cell transformation equally useful for dicotyledonous and monocotyledonous plants. The approach uses nitrate reductase-deficient mutants which cannot grow on nitrate as the sole nitrogen source, but can be propagated on reduced nitrogen sources such as amino acids, urea, or ammonia. These mutants provide a strong selection permitting the isolation of rare events. Genes coding for the molybdenum cofactor functions essential for nitrate reductase activity were isolated from Escherichia coli. Previous experiments showed that these genes code for functions which produce a product that can interact in vitro with the plant nitrate reductase apoprotein to regenerate a functional enzyme. These genes are being physically mapped with restriction enzymes and sequenced. The sequence information is important to combine the E. coli genes with a promoter functional in plant cells. The constructed chimeric plasmid will be introduced in the plant cells via liposomes and microinjection. Integration of the foreign gene into the plant cell genome will be facilitated by homologous recombination and transposable elements. The procedures developed will lead to genetic engineering of plants. This will in turn lead to the development of plants more suitable for biomass or specific product (oils, carbohydrates, proteins, secondary metabolites) production.

75. UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

STUDIES ON THE CONTROL OF PLANT CELL ENLARGEMENT BY CELLULAR PARAMETERS — $62,753

Robert E. Cleland
Department of Botany, KB-15

The goal of this research is to determine how plant cell enlargement is controlled and regulated at the cellular level by the hormone auxin. Previous studies have indicated that auxin causes cells to excrete protons into the cell wall, where the resulting acidic pH activates "wall loosening" processes. One part of our research concerns the nature of this wall loosening process. Isolated cell walls of the oat coleoptile, when under tension, extend in response to acid. We are characterizing this process in terms of its dependence on pH, tension, temperature, and prior history of the tissue. A second aspect of this research is to study the relationship between the energy metabolism of cells and the auxin-induced proton excretion. The short-term effects of auxin on nucleotide di- and triphosphates are being measured for the first time, and inhibitors are being used to probe the relationship between various types of respiration and proton excretion. Finally, the relationship between the turgor pressure of cells and the rate of cell enlargement is being studied by measuring turgor pressure directly with a micro-pressure probe under conditions where the growth rate is being varied. These results should provide us with a clearer understanding of the mechanisms which control cell enlargement in plants, and thus their primary productivity.

76. UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

THE FERMENTATION TO ETHANOL OF XYLOSE PRESENT IN BIOMASS BYPRODUCT SOLUTIONS — $92,000

Benjamin D. Hall, Mary Lidstrom, Clement E. Furlong
Departments of Genetics, SK-50 and Microbiology & Immunology, SC-42

The goal of this project is to develop a yeast strain that will fermentatively convert xylose to ethanol. Preliminary studies on the pentose fermentative pathway in the yeasts S. cerevisiae and S. pombe suggests an inability to isomerize xylose to xylulose. These yeasts can fermentatively utilize xylulose. In order to overcome the xylose isomerase deficiency, we are presently attempting to express the xylose isomerase gene of E. coli in these yeasts. Using a gene bank from an E. coli xylose positive strain, we have isolated a clone that complements the xylose isomerase defect of a xylose isomerase negative E. coli mutant. From this clone, we have isolated and determined the sequence of a 1.4 kb fragment of DNA that complements the xylose isomerase defect. In addition, we have purified to homogeneity the E. coli xylose isomerase, and determined the partial n-terminal amino acid sequence of this protein. Comparison of the protein and DNA sequence data conclusively proved that the clone contains the xylose isomerase structural gene. We have fused this gene to the promoter fragment of Adh 1 and Adh gene from S. cerevisiae and S. pombe respectively. The transcriptional and translational expression of the hybrid gene in these yeasts is being examined. Clones of S. cerevisiae and S. pombe that produce functional xylose isomerase enzyme will be analyzed for ethanol production. These yeast transformants will then be genetically manipulated in order to select mutants which will efficiently ferment xylose in spent sulfite liquor into ethanol.

77. UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

A STUDY OF THE GENETICS AND REGULATION OF METHANE OXIDATION — $49,712
Mary Lidstrom
Department of Microbiology and Immunology SC-42

The objective of this project is to study genetics and regulation of C-1 specific functions in methanotrophic bacteria. We have isolated and characterized the plasmids found in nine different obligate methanotrophs. They range in size from 26 to 120 Mdal, and are at present entirely cryptic. We have shown that they do not contain the structural genes for nitrogen fixation, and that they do not contain antibiotic resistance markers. DNA-DNA hybridization analysis has revealed homology only in the case of the plasmids from two different Methylosinus species, and only a small region of each plasmid is homologous. We have used a series of broad host range cloning vectors derived from pRK290 and a mobilizing plasmid (pRK2013) to move genes between methane and methanol utilizing bacteria. Our approach for the remainder of this project involves using cloned C-1 genes from facultative methanol utilizers to identify and isolate genes with similar functions in obligate methanotrophs. This work is of primary importance for the manipulation of methylotrophic bacteria for commercial chemical production.

78. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

DEVELOPMENT OF NITROGEN-FIXING MONOCOT-BACTERIA ASSOCIATIONS — $68,000 (FY 82 funds)
Winston J. Brill
Department of Bacteriology and Center for Studies of Nitrogen Fixation

The objective is to understand the ecology and physiology of nitrogen-fixing bacteria that associate with corn roots. With plants grown in the phytotron, an increase of nitrate concentration increases the rate of acetylene reduction by the associated bacteria. Most probable number estimations of Azospirillum-like bacteria showed that there was no significant differences between the numbers of nitrogen-fixing bacteria observed on roots of active versus inactive corn lines. Many unidentified bacteria are observed in the extracellular mucilage, and typically have an electron-lucent zone surrounding them. Bacteria are seldom seen in epidermal cells, and rarely in cortical cells. The location of the bacteria suggest that the primary site of colonization is the epidermal slime layer, not the interior of the root, as has been postulated by most investigators. It is hoped that manipulation of these microbes and the host plant will allow plants, such as corn, to obtain a significant percent of their required nitrogen from atmospheric nitrogen through associative nitrogen fixation.

79. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

ORGANIZATION OF THE R CHROMOSOME REGION IN MAIZE — $41,306
Jerry L. Kermicle
Laboratory of Genetics

We seek to identify and map components of the R gene in corn which govern the presence, distribution and timing of anthocyanin pigmentation. A simplex R allele (not duplicated) is composed of a tissue specific segment of short genetic length and a longer segment that is common to alleles of different tissue specific activities. This inference derives from three mutations induced by the transposable element Dissociation, (Ds), analyzed in recombination tests with alleles of contrasting tissue specific effects. This analysis is being extended to include spontaneous and chemically induced mutants as well as to a larger group of Ds variants. Components underlying a heritable interaction between alleles (paramutation) are being mapped similarly. We want to relate the genetic components responsible for tissue specific control to those responsible for paramutations.

80. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

STARCH SYNTHESIS IN THE MAIZE ENDOSPERM AS AFFECTED BY STARCH-SYNTHESIZING MUTANTS — $55,430
Oliver E. Nelson
Department of Genetics

Our objective in this project is to utilize the numerous mutants of maize to gain increased knowledge of the important process of starch biosynthesis in cereal seeds. During the past year, we've been able to establish that the sugary mutant of maize (the usual sweet corn of commerce) whose principal carbohydrate storage product is not starch but the highly branched water-soluble polysaccharide, phytoglycogen, lacks a debranching isoenzyme [an α-(1-6)-glucosidase] present in nonsugary endosperms. This suggests that the amylopectin component of starch is the result of an equilibrium between enzymes introducing α-(1-6) linkages into starch and enzymes cleaving those linkages. We have also detected the existence in developing maize endosperms of two oligosaccharide synthases--enzymes capable of synthesizing short chain length maltodextrins from glucose-1-PO_4. These oligosaccharide synthases may be responsible for the primers which all starch synthases require to function and hence would carry out the initial step of starch synthesis.

81. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

CARBON ISOTOPE FRACTIONATION IN PLANTS — $71,593
Marion H. O'Leary
Departments of Chemistry and Biochemistry

Plants fractionate carbon isotopes during photosynthesis in ways which reflect photosynthetic pathway and environment. The object of our work is to develop methods for using this isotope fractionation to give information about how the components of the carbon fixation process (diffusion, carboxylation, etc.) vary with species, environment, and other variables. To this end, we have developed quantitative models for carbon isotope fractionation which describe this process in terms of rates of diffusion, carboxylation, and other components. We have developed experimental approaches which focus on the initial events in carbon dioxide fixation and enable us to determine the relative rates of the various individual processes involved. During the current project period (June, 1983), we have been analyzing malic acid samples obtained from plants showing Crassulacean acid metabolism following nocturnal exposure of these plants to $^{13}CO_2$ or $^{13}C^{18}O_2$. From these samples we will determine the activity of carbonic anhydrase in these plants and we will determine the extent to which fumarase randomizes malate during nocturnal CO_2 fixation.

82. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

PHYTOCHROME FROM GREEN PLANTS: ASSAY, PURIFICATION AND CHARACTERIZATION — $50,000
Peter H. Quail
Botany Department

The objective of this project is to purify and characterize the phytochrome molecule(s) from light-grown chlorophyllous tissue of higher plants and algae. The approach involves the use of (a) purification procedures that greatly reduce chlorophyll levels (principally polyethyleneimine precipitation) to permit spectral analysis, and (b) immunological procedures for further characterization. The difference spectrum of the phytochrome from green Avena is distinct from that of phytochrome from etiolated shoots in that the Pr maximum is shifted to shorter wavelengths. Immunoprecipitation of 'green' phytochrome with antibodies directed against 'etiolated' oat phytochrome distinguishes two populations of spectrally active phytochrome. 25% of the 'green' phytochrome is recognized by this IgG, but requires 2.5-fold more IgG than for 'etiolated' phytochrome to maximize immunoprecipitation; the remaining 75% is not recognized. Mixing experiments indicate that these apparent immunochemical differences between 'green' and 'etiolated' phytochrome are neither the result of posthomogenization modifications nor of interfering substances in the green tissue preparations. The significance of these data is that they suggest the presence in cells of light-grown tissue of one or more phytochrome species distinct from the well-characterized molecule that predominates in etiolated tissue. Together with the absence of detectable levels of immunoprecipitable phytochrome apoprotein among the in vitro translation products of poly(A) RNA from green tissue (Proc. Natl. Acad. Sci. US 80: 2248, 1983), these data suggest the possibility of more than one phytochrome gene.

83. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

MOLECULAR MECHANISM OF ENERGY TRANSDUCTION BY PLANT MEMBRANE PROTEINS — $61,440

Michael Sussman
Department of Horticulture

The focus of this project is a protein that converts chemical energy into electrical energy. This protein is known as a $[H^+]$-ATPase, or proton pump, and is found in the plasma membrane of fungi and higher plants. Its function is to generate a proton electrochemical gradient across this membrane. The gradient is mainly an electrical potential which, in root hair cells of higher plants and hyphal cells of mycelial fungi, can exceed 200 to 250 millivolts, interior negative. In these cells it generates a protonmotive force that is essential for the uptake of minerals and nutrients. This protein has unique molecular properties. Since it contains a single polypeptide of M_r=104,000 that is phosphorylated during the reaction cycle, its chemical structure is very similar to that of cation-translocating ATPase's found in the plasma membrane of animal cells (e.g., the NaK-ATPase of kidney, the HK-ATPase of stomach and the Ca-ATPase of muscle). However, since it only translocates protons, it is functionally more similar to the membrane ATPase found in bacteria, mitochondria and chloroplasts.

In this project, protein modification and sequencing techniques are used to study how the enzyme functions. Radioactive probes that react covalently with essential amino acids are used to characterize the enzyme's two active sites: (1) an ATP-binding site and (2) an ion-binding site. The primary structure of these sites will be determined by application of automated solid phase sequencing techniques. Essential amino acids will be further identified by comparing the amino acid sequence obtained with enzyme isolated from many plant species. Results derived from the study of this unique protein will be used to define a molecular mechanism for protein-mediated energy transduction.

84. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

ONE CARBON METABOLISM IN ANAEROBIC BACTERIA: ORGANIC ACID AND METHANE PRODUCTION — $106,000

J. Gregory Zeikus
Department of Bacteriology

This research aims to identify the pathways and regulation of carbon and electron flow during one carbon metabolism by acetogenic and methanogenic bacteria. The approach involves comparison of growth parameters, enzyme activities and end products formed in relation to the fermentation of H_2-CO_2, HCOOH, CO, CH_3OH and acetate. Emphasis is placed on determination of the biochemical mechanism of acetate synthesis from one carbon compounds or the synthesis of methane from acetate by specific carbon tracer analysis (i.e., ^{14}C, ^{13}C-NMR, and ^{18}O), enzymatic analysis (i.e., one carbon oxidoreductases, such as CO dehydrogenase) and mutant analysis (i.e., metabolic lesions in one carbon transformation reaction). The results are of importance to biotechnology because acetic acid is a major chemical commodity and methane is a major fuel source.

43

85. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

BIOCONVERSION BY PHOTOSYNTHETIC SYSTEMS — $85,000
John L. Bennett

The objective of the research is to determine the effects of environmental factors on the structure, function and formation of chloroplasts of plants and algae. Adaptive control mechanisms are being sought in these systems. Three areas of control are being explored: (1) regulation of chloroplast formation at the levels of gene transcription and protein turnover, (2) homeostatic control of photosynthetis by reversible phosphorylation of chloroplast proteins, and (3) adaptation of the photosynthetic apparatus to extreme environmental conditions through mechanisms involving the regulation of gene expression and/or post-translational controls. Although special emphasis will be given to light as an environmental variable (including changes in light intensity, spectral quality and daily duration), the modifying effects of high and low temperature, water stress and disease will also be studied. Current studies of the regulation of gene transcription involve the use of cloned DNA probes prepared against the gene for major chloroplast proteins such as ribulose bisphosphate carboxylase/oxygenase and the light-harvesting chlorophyll a/b protein (LHCP). In the future it is hoped to include genes for other chloroplast proteins in the study. Current aspects of research on chloroplast protein phosphorylation include the regulation of excitation energy distribution within thylakoids by the reversible phosphorylation of LHCP, the control of PSII activity by the phosphorylation of PSII polypeptides, the regulation of cyclic and non-cyclic electron transport, and the regulation of CO_2 fixation. Emphasis is being given to the purification of the protein kinases, both thylakoid-bound and soluble, which play central roles in these regulatory phenomena.

86. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

PLANT MOLECULAR GENETICS — $200,000
Benjamin Burr and Frances A. Burr

The primary research project of the laboratory has been an investigation of the molecular structure and genetic characteristics of maize transposable elements. The major portions of one large element, Dissociation (Ds), have been cloned. This particular receptor element is over 20,000 bp in length. The segments cloned include the important junction regions between the insertion and the wild-type sequences. Using the clones as hybridization probes, we have deduced that at least part of the Ds insertion is not repeated in the genome. Based on genetic evidence, Ds had been anticipated to be present in multiple copies. By careful analysis of several Ds mutations at the Shrunken locus, we have found that the structure of Ds can differ significantly. We believe that these differences are the result of structural rearrangements that the element undergoes in the process of transposition or while at a fixed position, the latter being responsible for a "change-of-state" of the phenotype. We have also been working with another transposable element family in maize called Mutator. These elements are genetically distinct from the controlling elements described by McClintock. Two Mutator (Mu) elements have been cloned and their structures analyzed. One of these is detected only in strains possessing Mutator activity and, in contrast to Ds, it appears to be a stable structure. These characteristics suggest that it would be an ideal element to use for isolating genes by transposon tagging. Mutants at a number of loci have been obtained using Mutator. The Mutator cloned from the Shrunken locus is currently being used as a probe to select random clones from strains with Mutator at the Bronze locus.

87. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

MECHANISMS OF ENERGY CONVERSION IN PHOTOSYNTHESIS — $270,000
Geoffrey Hind
Biology Department

The goal of this project is to discover how energy is transformed from electron potential to chemiosmotic potential in photosynthetic systems. Processes involving cyclic electron transport are of prime concern and are studied in (1) intact chloroplasts of the C-3 plant, Spinacia oleracea, (2) bundle sheath cells of the C-4 plant, Zea mays and (3) isolated heterocysts from the filamentous cyanobacterium Anabaena 7120. In these systems, electron flow from reduced plastoquinone to the photochemically generated oxidant, $P700^+$, is mediated by a cytochrome b/f complex. The polypeptide compositions of complexes from these organisms are being compared and their activities in situ or following detergent extraction are being studied using flash, steady state and low temperature spectrophotometry. Special interest attaches to the means by which, in cyclic flow, electrons return to the cytochrome complex from the strong reductant generated by photosystem 1. Passage of electrons through the complex is coupled to vectorial H^+ transport, possibly by a form of "Q-cycle" as postulated by Mitchell; the stoichiometry of this coupling and its dependence on ambient redox poise are being studied to elucidate the coupling mechanism. The source of reductant needed to poise the cycle is also of concern; in C-3 photosynthesis, activity of photosystem 2 is normally adequate to poise the cycle and the problem is rather to ascertain what mechanisms are involved in preventing total inhibition of cyclic flow by competition with non-cyclic reductions of $NADP^+$ and O_2. These investigations will provide knowledge of the factors limiting photosynthetic reduction of CO_2 and N_2. In showing how the cytochrome complex serves as an efficient energy transformer, they are also of presumed relevance to future design of biomimetic energy conversation devices.

88. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

THE REGENERATION OF PLANTS FROM CROWN GALL TUMORS — $140,000
Daniela Sciaky
Biology Department

The genetic engineering of plants using the T-DNA of Agrobacterium tumefaciens requires that the engineered plant cell be regenerated into a fertile plant. Two separate occurrences are being studied with respect to understanding how crown gall callus can organize into shoots. One event is the spontaneous formation of shoots from Nicotiana otophora cells transformed by pTi86806. The T-DNA in these shoots is no longer colinear with the T-DNA of undifferentiated transformed cells. Fragments of T-DNA from the shooting tumors will be isolated to determine how the T-DNA is organized in these tumors and to understand how the T-DNA was rearranged. The second event is the localization of a 2.7 kb insert in the T-DNA of pTiA66 leading to the requirement for auxin to induce tumors in some plants. When these tumors are placed in tissue culture they sometimes form shoots and lose their auxin requirement. Sequences homologous to the 2.7 kb insert are present in other regions of the Ti plasmid of A66 and in the A66 chromosome. The primary structure of the junction between the insert and T-DNA indicates that the insert has the structure of a transposable element. Studies are being initiated to determine whether this structure can act as a transposable element in plants and, how this structure regulates the appearance of shoots in tumors.

89. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

THE PHYSIOLOGY AND BIOCHEMISTRY OF CYANOBACTERIA — $185,000
Harold W. Siegelman
Biology Department

The organism Microcystis aeruginosa is probably the most successful cyanobacteria in freshwaters, and it occurs worldwide. It is usually responsible for algal blooms and may cause serious water management problems. The success of the organism is probably associated with an efficient photosynthetic mechanism and a gas vacuole system which permits vertical movement in the water column. The molecular structure and composition of the photosynthetic energy collection systems including phycobilisomes, chlorophyll, carotenoids, and reaction centers are being characterized in several strains. The cells grow successfully over a very wide range of light intensities. The effects of light intensity are being examined with turbidostat and low cell density cultures. Phycobilisomes from cells grown at several light intensities are characterized by agarose cell filtration, hydrophobic-interaction chromatography, electron microscopy, phycobiliprotein stoichiometry, and fluorescence and absorbance spectroscopy. The cell walls of two widely-separated geographic strains have different compositions and additional strains are being examined. The number and composition of the pentapeptide toxins of M. aeruginosa are strain specific, and their biosynthesis is inversely related to cell division rate. The toxin structures are being determined by amino acid analysis and mass spectroscopy. Pathological and hematological studies indicate that the toxins require an in vivo activation process and then cause thrombocytopenia. The toxicity is apparently due to pulmonary thrombosis. The lipid and carbohydrate composition of several strains of M. aeruginosa are being examined by chromatographic and mass spectral methods. The compositional analysis of several strains of M. aeruginosa for lipids, carbohydrates, carotenoids, and toxic pentapeptides may provide a useful basis for strain identification or classification of morphologically-similar isolates of a single species. These components may provide useful intermediates for chemical feedstocks.

90. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

PLANT CELL GENETICS — $20,000
Harold H. Smith
Biology Department

The objective of this project is to gain an understanding of genetic controls in plant development through cell and tissue culture and the analysis of genetic tumors. The genetic basis of spontaneous tumor formation in certain Nicotiana plants is being studied by isolating particular chromosomes that, when transferred to distantly related species, cause tumors to develop. These chromosomally-defined, tumor prone plants are being grown in tissue culture to determine their differences from normal plants in growth factor requirements, and with regard to differences in superoxide dismutase, an enzyme characteristically deficient in mammalian tumors. Transmission genetics of the alien tumor-controlling chromosome, from the fourth to the ninth segregating generation, reveals that: (1) about half the plants produced by self pollinating such 2n+1 plants have the extra chromosome (a nigh rate of transmission), and (2) only about half the plants with this extra chromosome actually form tumors (a low rate of penetrance). The total enzyme activity of superoxide dismutase is found to be as high in these tumorous genotypes as in the nontumorous ones, a result that is contrary to findings with many animal tumors. The Nicotiana tumor system provides a unique material for further studies on genetic controls of differentiation.

91. LAWRENCE BERKELEY LABORATORY
Berkeley, CA 94720

RESONANCE STUDIES IN PHOTOSYNTHESIS — $60,000
Alan Bearden
Donner Laboratory

The first objective of this work has been the further study of the role of iron-sulfur proteins in the acceptor structure of chloroplast Photosystem I. Studies by low-temperature electron paramagnetic resonance (EPR) spectroscopy with partially oriented membranes from the green halophilic alga, Dunaliella parva have shown the existence of an iron-sulfur cluster with an orientation different from the previously known acceptors, Cluster A and Cluster B. Concomitantly time-resolved EPR spectra of whole chloroplasts and photosynthetic particles isolated with enhanced Photosystem I activity, clearly indicate a more complicated set of early reaction in the primary/secondary dynamics of this Photosystem. Preliminary publication of these results has been in Biochimica Biophysica Acta 720-722, 16-19 (1983) and 723, 23-25 (1983). Secondly, we have completed during this fiscal year the first experimental demonstration of "Hopfield" charge transfer band arising from tunneling processes in the electron-transfer in the photosynthetic bacterium, Chromatium. These results have been accepted for publication in the Proceedings of the National Academy of Sciences. The generality of these latter studies to problems in biophysics and solid state physics has been recognized and a first paper has been published in the Physical Review B 27, 7431-7439 (1983); papers for Physical Review Letters and the Journal of Molecular Biology are in preparation.

92. LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
Berkeley, California 94720

PHOTOCHEMICAL CONVERSION OF SOLAR ENERGY — $110,000
Lester Packer, Rolf J. Mehlhorn, Alexander T. Quintanilha
Membrane Bioenergetics Group, Applied Science Division

This program seeks to characterize the molecular events associated with photochemical conversion mechanisms. Bacteriorhodopsin is a light- and temperature-stable protein, which operates via a photocycle to develop a proton current, contains retinal as a chromophore, and is the only protein found in the purple membrane isolated from Halobacterium halobium. Chemical modification and electron spin resonance techniques will be used to study the topography of carboxyl residues of bacteriorhodopsin. We seek to characterize buried carboxyl groups located in hydrophobic protein domains near the retinal chromophore, and at least 16 Å from the membrane surface, and on the carboxyl-terminal tail, and to determine whether modification of these groups perturbs the light-induced proton pumping activity. The data will be compared with several models of bacteriorhodopsin's tertiary structure to determine if, like other membrane proton pumps, a buried carboxyl group is required for activity.

93. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

CELL CYCLE DEPENDENT EXPRESSION OF GENES CODING FOR PHOTOSYNTHETIC PROTEINS IN EUGLENA GRACILIS — $28,000

James C. Bartholomew
Chemical Biodynamics Division

In this project we will map the genes coding for photosynthetic proteins in Euglena gracilis into the nuclear or chloroplast domain. Plasmids containing DNA homologous to mRNA's for reaction center proteins will be used to study the regulation of expression of the photosynthetic genes during the cell cycle and during plastid development. We will use in vitro translation systems to study the factors that effect the synthesis of these proteins. We hope to develop from these studies an understanding of how the genetic information coding for the photosynthetic apparatus is organized and controlled during plastid development.

94. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

PLANT BIOCHEMISTRY: REGULATION OF PHOTOSYNTHETIC METABOLISM AND SECONDARY BIOSYNTHESIS — $280,000

James A. Bassham
Chemical Biodynamics Division,

The objectives of this project are to determine photosynthetic and biosynthetic paths in green plants and the mechanisms of regulation in these paths. Both metabolic regulation (feedback inhibition, energy charge, etc.) and regulation of gene expression are studied in plant tissue, including whole plants and organs, cells and organelles isolated from leaves, and plant tissue culture. Subtask I (Regulation of Metabolism and Gene Expression) focuses on key enzymes and processes of metabolism in photosynthetic cells, and is directed to obtaining a better understanding of control of primary carbon and nitrogen metabolism in these cells, including specialized cells found in certain plants (C_4 plants). Subtask II (Secondary Plant Metabolism: Plant Pigments) includes similar goals focussed on secondary products and also investigation of structures and mechanism of action of non-chlorophyllous plant pigments.

95. LAWRENCE BERKELEY LABORATORY and the
UNIVERSITY OF CALIFORNIA, BERKELEY
Berkeley, California 94720

MAPPING PHOTOSYNTHETIC GENES IN RHODOPSEUDOMONAS CAPSULATA — $82,000
John E. Hearst
Department of Chemistry and the Laboratory of Chemical Biodynamics

The objectives of this project include the mapping and sequencing of light harvesting and reaction center genes in Rhodopseudomonas capsulata. The regulation of these genes and a study of their phylogenetic relationship to similar genes in other photosynthetic bacteria, algae and higher plants are anticipated. In this fiscal year, five structural genes coding for the reaction center (RC) L, M and H subunits and the two light harvesting (LH) I polypeptides, LHP1 and LHP2, have been mapped on two restriction fragments from the R-prime plasmid, pRPS404. The genetic map of the R-prime plasmid has been aligned with the restriction map. It had been shown that enhanced near-infrared fluorescence mutants of R. capsulata typically lack RC or LH I polypeptides and that these lesions are marker rescued by two restriction fragments from the R-prime plasmid: the 7.5 kb Eco F fragment and the 4.75 kb Bam C-Eco B fragment. We have now determined the nucleotide sequence of these two restriction fragments and have found that the Bam C-Eco B fragment carries the structural genes for the RC L and M subunits and both LH I polypeptides. Thirty kilobasepairs (kb) away from this locus, the Bam F fragment (within the Eco F fragment) carries the RC H subunit.

96. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

WATER SPLITTING AND OXYGEN EVOLUTION IN PHOTOSYNTHESIS — $105,000
Melvin P. Klein
Chemical Biodynamics Division

The details by which manganese participates in the photosynthetic oxygen evolution reactions are obscure. Our efforts in this area are directed at the use of X-ray spectroscopy, low temperature EPR and Electron Spin Echo spectroscopy to extract structural information about the manganese centers of photosynthetic membranes. These structural parameters and the changes that occur during function of the membrane apparatus are to be used as a framework for the elucidation of mechanistic details of the water splitting process. Previous studies using X-ray absorption techniques in our laboratory have provided information about the ligand structure and average oxidation state of manganese in active dark adapted (resting) photosynthetic membranes. Significant advances have recently been made in that stable, active sub-chloroplast membrane preparations from spinach containing only the photosystem II light reactions are now available. Secondly, a photo-induced EPR signal rich in manganese hyperfine structure has recently been observed at low temperature in chloroplast preparations and is interpreted as arising from reactions close to the oxygen evolving complex. X-ray spectroscopic data of these same preparations indicates an oxidation and ligand state of manganese distinctly different from that of dark adapted membranes.

49

97. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

STUDY OF THE STRUCTURE AND MECHANISM OF ACTION OF PHYTOCHROME — $82,000
Henry Rapoport
Department of Chemistry, University of California

The objectives of this project are to study the structure and mechanism of action of the non-chlorophyllous plant protein-pigment phytochrome. Phytochrome is the morphogenically active plant pigment which controls all developmental aspects of plant growth. It does this by undergoing a photochemical interconversion upon light excitation to a new, active form. The specific structural features of this isomerization, as well as some other structural aspects of phytochrome, remain unknown. It is essential that these structural questions be unambiguously established in order to have a full understanding of phytochrome's function. Understanding the underlying mechanism by which phytochrome functions as a reversible biological switch may allow us to control growth, flowering, and fruiting. The action of far red light causes phytochrome to change from the inactive P_R form to the active P_{FR} form. The two most reasonable hypotheses for its mode of action in the P_{FR} form are through gene activation or by affecting membrane permeability. However, structural information on exactly what changes accompany the transformation to the P_{FR} form is totally lacking. We plan to provide this information by applying detailed NMR analysis to this transformation.

98. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

CHARGE SEPARATION IN PHOTOSYNTHETIC LIGHT REACTIONS — $168,000
Kenneth Sauer
Chemical Biodynamics Division

We are using electron paramagnetic resonance spectroscopy (EPR) and fluorescence lifetime measurements to monitor the dynamics and mechanism of charge separation associated with the primary light reactions of photosynthesis. Transient EPR measurements exhibit electron spin polarization that reflects the chemical nature of the molecular species involved as well as their distance of separation and their orientation in the photosynthetic membranes. Fluorescence decay kinetic studies elucidate the pattern of excitation transfer among the light-harvesting chlorophyll molecules and charge recombination in the reaction centers. Analysis of the several exponential decay components shows that they can be distinguished with respect to their response to excitation intensity, added redox agents, divalent cations and conditions that result in membrane phosphorylation. In addition to providing knowledge about the electron carriers involved, these studies are informative about the membrane organization and how it is subject to control by secondary constituents.

We are also investigating the structure of reaction center complexes of photosynthetic bacteria. We have isolated the reaction center proteins from Rps. capsulata and are sequencing oligopeptides derived from them by selective cleavage. We are preparing to crystallize these complexes for detailed structure determination.

99.. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ANALYSIS OF PHOTOSYNTHETIC MEMBRANES — $219,000
C.J. Arntzen
MSU-DOE Plant Research Laboratory

Chloroplast membranes are the site at which the energy trapped from light during photosynthesis is converted into the stable chemical intermediates $NADPH_2$ and ATP. The photosynthetic light reactions require the concerted interaction of pigments that sensitize the process as well as electron carriers and enzymatic proteins. A central theme of this task is to understand the structural organization of the chloroplast membranes, which allows us to understand compartmentalization of individual functions and ultimately the regulation of efficiency and activity of the overall process. The approaches used in this research include ultrastructural analysis of developing and mature membranes, detergent fractionation of isolated membranes to isolate individual chloroplast membrane components, and characterization of both light-harvesting and electron transport partial reactions in the intact membranes or membrane subfragments. Current research emphasis is being directed upon the covalent modification of light-harvesting pigment-proteins via protein phosphorylation. The phosphorylation is involved in regulating the efficiency of energy trapping via the antennae pigment bed. We are currently testing the concept that this regulatory process involves the lateral mobility of a specific pigment-protein complex within various distinct regions of the chloroplast membrane system. We are also characterizing the functional activity of the photosystem II complex, with special attention being directed at the reaction center polypeptides and those polypeptides which appear to participate in the removal of electrons from water. The long term objective of this research program is to identify mechanisms which control the quantum efficiency of photosynthesis with the idea that understanding of these controls will allow us to successfully manipulate the photosynthetic process to optimize biomass productivity.

100. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

DIFFERENTIAL GENE EXPRESSION IN RHIZOBIUM — $157,000
Barry Chelm
MSU-DOE Plant Research Laboratory

The interaction of bacteria of the genus Rhizobium with a legume host to establish a symbiotic, nitrogen-fixing relationship requires a series of developmental steps in both the bacterium and the host plant. The objective of this project is to identify the underlying molecular mechanisms by which the expression of the bacterial genome is regulated during this process. We have focused primarily on the R. japonicum/soybean system. Specific genes whose expression is regulated during nodule development or by other physiological changes have been isolated by hybridization screening of an R. japonicum DNA fragment library carried in an E. coli phage lambda vector. The genes isolated thus far include those encoding the nitrogenase subunits, glutamine synthetase I and the large subunit of ribulose bisphosphate carboxylase. The expression patterns and structures of these genes are being further characterized. Promoter regions are being localized by S1 protection analysis and the nucleotide sequences of these regions are being determined. Other developmental stage specific R. japonicum genes are being isolated through the use of stage specific hybridization probes. These stage specific probes are being prepared from total genomic DNA by first removing sequences which are present in other cell types via RNA excess hybridization followed by RNA saturation with RNA from the developmental stage of interest and will be used to characterize the stage specific RNA population in detail by kinetic analyses and to isolated stage specific genes from genomic libraries. The isolated genes will be genetically manipulated and reintroduced into rhizobia in order to establish the importance of these genes for the process of nodulation. These further understandings of the processes regulating legume nodulation and nitrogen fixation should enlighten the viewpoint from which the symbiotic relationship might be further optimized.

101. MICHIGAN STATE UNIVERSITY,
East Lansing, Michigan 48824

RESISTANCE OF CROP PLANTS TO ENVIRONMENTAL STRESS — $94,000
Andrew D. Hanson
MSU-DOE Plant Research Laboratory

This project seeks to identify metabolic pathways which are activated by environmental stress and which have adaptive significance, and to understand the genetic and environmental control over these pathways. The aim is to use natural or induced genetic variation in the expression of such adaptive pathways in breeding stress-resistant crops. (1) Anaerobic stress and glycolytic pathways in imbibed barley aleurone and embryo tissues. These seed tissues -- unlike other tissues of the barley plant, -- can withstand complete anoxia for several days, during which both lactate dehydrogenase (LDH) and alcohol dehydrogenase (ADH) activities are induced and lactate and ethanol accumulate as glycolytic end-products. Both LDH and ADH systems are being subjected to isozyme and immunological analysis, as first steps in characterizing their genetic and environmental regulation. (2) Betaine accumulation in barley. Natural variability for the activity of the stress-induced betaine synthesis pathway has been surveyed in wild and cultivated barley. The available diversity found (a two- to three-fold range) has proven adequate for inheritance studies which have shown the betaine trait to be highly heritable. Accordingly, a program has been started to develop isopopulations, low and high in betaine, for a direct test of the value of high betaine levels in stressed field environments.

102. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ACTION AND SYNTHESIS OF PLANT HORMONES — $219,000
Hans Kende
MSU-DOE Plant Research Laboratory

The principal objective of this task is to gain knowledge on the mode of action of the plant hormones ethylene and cytokinin. These hormones regulate processes related to stress and senescence in plants. Ethylene promotes aging and the appearance of stress symptoms, cytokinins retard them.

a) Regulation of stress-ethylene synthesis. Plants under stress produce ethylene. Ethylene synthesis is very rapidly induced through the enhancement of the activity of 1-aminocyclopropane-1-carboxylate (ACC) synthase. This enzyme is de novo synthesized during induction of ethylene synthesis. Research will mainly concentrate on the mechanism by which ACC synthase is regulated. Antibodies against ACC synthase will be produced for the isolation and further characterization of the enzyme. Using these antibodies, we shall also study the level of control of this enzyme and the mode of its turnover. We are also studying the role of stress ethylene in rice plants. When rice is flooded, it perceives this as a stress and synthesizes ethylene in response to it. Ethylene induces growth in rice and permits it to maintain its foliage above the water. We are investigating the mechanism by which ethylene, perhaps in conjunction with other growth regulators, controls growth in rice plants.

b) Localization of the site of action of cytokinins. We are synthesizing a cytokinin photoaffinity probe, 8-azido-N^6-benzyladenine, in radioactive form to localize the site of action of this hormone. This will be attempted using two plant systems: moss protonemata and cultured tobacco cells. Cytokinins induce bud formation in mosses and are accumulated by target cells of this organism. In tobacco cells, cytokinins regulate cell division. We shall attempt to isolate the tagged receptor from both types of cells in order to characterize it and localize it in the cell.

103. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

CELL WALL PROTEINS — $124,000
D.T.A. Lamport
MSU-DOE Plant Research Laboratory

Our major objective is to determine the function of extensin, a hydroxyproline-rich cell wall glycoprotein of higher plants. Recently we proposed a new model of the cell wall consisting of two concatenated polymeric systems: a cellulose "warp" interpenetrating a crosslinked extensin "weft". Such mechanical coupling between two polymers provides a new basis for understanding cell extension. Current approaches involve (i) isolation of two precursors (P1 and P2) of the firmly bound structural protein extensin from tomato cell suspension cultures. (ii) Structural elucidation of the possible role of the crosslinked amino acid isodityrosine (IDT) in extensin. (i) We propose to characterize the precursors kinetically, compositionally and electron microscopically. Kinetic experiments will involve pulse-chase experiments followed by isolation of the labelled precursors to determine turnover rates at different stages of growth. This will help distinguish between possible rate-limiting steps in wall assembly; secretion or attachment. We propose to peptide map and sequence P1 and P2 as an approach to a determination of their relationship, and function. Sequence data will help to predict IDT crosslink domains and hence determine network size and porosity predicted by the new cell wall model. Electron microscopic approaches will help define those network parameters which depend on IDT crosslinkages. (ii) We shall attack the questions of IDT crosslinkages by isolation of small multimers of extensin. We predict these are formed (a) during the attachment process in muro, and (b) by an in vitro peroxidatic crosslinkage system to be developed.

104. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

REGULATION OF FLOWERING — $94,000
Anton Lang
MSU-DOE Plant Research Laboratory

This project deals with the regulation of flower formation by hormone-like (i.e. translocatable) substance, the main focus currently being on inhibitors of flower formation ("antiflorigen"). The existence of antiflorigen in some long-day plants has been conclusively demonstrated, in previous research on this project, by grafting experiments with species of Nicotiana and Hyoscyamus. Antiflorigen, like the promotive hormone-like factor(s) of flower formation ("florigen, floral stimulus"), is not specific in either the taxonomic or the physiological sense, being interchangeable between different species and genera, and between plants in which flowering is dependent on different environmental (photoperiod) requirements. This physiological evidence argues strongly that both antiflorigen and florigen are ubiquitous in flowering plants. The next logical step is isolation and chemical identification of these agents. We are currently working on this problem, with emphasis on antiflorigen since - among various reasons - solution of this problem may be helpful in the search for florigen which so far has been unsuccessful. For isolating antiflorigen, we are using both solvent extraction and phloem diffusion, for assay mainly explants from tobacco inflorescence stems which initiate flower buds in vitro. Continued grafting experiments have indicated that our principal shortday plant (Maryland Mammoth tobacco) does not seem to produce antiflorigen, at least not in the amounts produced by the long-day plants mentioned above.

105. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

THE MOLECULAR-GENETIC BASIS FOR THE DEVELOPMENT OF PHOTOSYNTHETIC COMPETENCE — $157,000
Lee McIntosh
MSU-DOE Plant Research Laboratory

The aim of this research project is to delineate the molecular-genetic basis of photosynthetic competence in higher organisms and to genetically modify specific polypeptides involved in photosynthesis. To accomplish these goals we are (1) isolating chloroplast and nuclear genes whose products are integral photosynthetic components, (2) investigating the regulatory regions of the genes and functional domains of their products, and (3) employing gene mutations to artificially alter photosynthetic capacity in the transformable photosynthetic system. The first two chloroplast gene mutations we are characterizing are those which transmit resistance to streptomycin and the herbicide atrazine. Our recent results indicate that resistance to atrazine appears to be due to a single amino acid substitution in the primary sequence of a 32 Kilodalton (Kd) thylakoid membrane polypeptide. The 32 Kd herbicide binding protein has also been shown to display lower efficiency of electron transport in several species of weeds with atrazine resistant biotype. We intend to employ the mutant "resistance" gene to transform the naturally transformable cyanobacterium Synechococcus R2. The purpose of these experiments is to introduce a chloroplast gene into cyanobacteria and to test for functional integration of the foreign gene product into the photosynthetic apparatus. We are also investigating the possibility of altering (reducing) photorespiration - the net inhibition of photosynthesis due to oxygen competition with CO_2 at ribulososebisphosphate carboxylase (rubisco) - by the direct alteration of the gene encoding the catalytic (large) subunit of rubisco. Our first approach is to employ the bacterial large subunit gene from Rhodospirillum rubrum which is cloned, expressed and functional in E. coli. We have completed the DNA sequence of the gene and are now changing specific bases within the gene to give site-specific amino acid substitution.

106. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

SENSORY TRANSDUCTION IN PLANTS — $141,000
Kenneth L. Poff
MSU-DOE Plant Research Laboratory

The objective of this project is to understand the mechanism whereby plants sense the state of their environment through the perception of light and temperature. Light is sensed by two major systems in plants: the blue light photoreceptor pigment, and phytochrome. We are studying phytochrome through a continued selection for and physiological characterization of mutants with altered pathways for the production of phytochrome and for its utilization. The blue light photoreceptor pigment regulates phototropism through which light direction is measured. For such a measurement, a gradient in light intensity must exist through the organism. Mutants and inhibitors are being used in corn, sunflowers, and soybeans to distinguish between a gradient produced via focusing and one produced via screening.

Thermotaxis in Dictyostelium discoideum is being used as a model system in an attempt to understand the mechanisms whereby an organism measures temperature or fluctuations in temperature. We can now demonstrate thermotaxis by the individual amoebae and, based on the physiological characterization of this response and on the response of several mutants, can conclude that slug thermotaxis is a manifestation of the thermotactic response of the component amoebae. Thus, we can safely ignore the organizational complexities of the multicellular slug and search for the "biothermometer" at or below the cellular level.

An understanding of photosensory transduction in plants is of importance since this environmental sensing preceeds and ultimately regulates photosynthetic capacity. Knowledge of thermosensing is of critical importance because of the major thermal limitations on plant productivity and the fact that heat is the ultimate product of any energy production and utilization.

107. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

IDENTIFICATION OF POSSIBLE TARGETS FOR GENETIC ENGINEERING IN PLANTS — $157,000
C.R. Somerville
MSU-DOE Plant Research Laboratory

The overall objective of this task is to develop genetic systems for the analysis and modification of specific physiological processes in plants. We are using this approach to investigate three separate areas of plant biology in which single gene variation may be a strong determinant of plant productivity.

A) Based on the premise that photorespiration is deleterious to plant productivity we are attempting to create useful or informative variation in the responsible enzyme by modifying the corresponding gene in vitro. We are also attempting to resolve several problems in our understanding of photorespiratory metabolism by the isolation of specific classes of mutants which have eluded discovery, and by characterization of a CO_2-concentrating mechanism by which some algae avoid photorespiration.

B) Disease is a major factor in yield of many crop species. Although genetic variation in disease resistance is available in most crop species, it is not known what "disease resistance" genes encode. We are exploring the possibility that novel immunological techniques (monoclonal antibodies) can be used to characterize the biochemical basis of the genetic differences between disease resistant and susceptible cultivars of soybeans. Identification of responsible factors would permit rational assessment of disease management strategies and novel approaches to genetic manipulation of the resistance genes.

C) Many species of economic importance are extremely chilling sensitive whereas related species are often quite tolerant of chilling temperatures. We are exploring the mechanisms involved in chilling resistance by the isolation and biochemical characterization of single gene mutations which dramatically alter the chilling sensitivity of a model plant (Arabidopsis thaliana).

108. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

DEVELOPMENTAL BIOLOGY OF NITROGEN-FIXING ALGAE — $157,000
C.P. Wolk
MSU-DOE Plant Research Laboratory

Certain cyanobacteria (blue-green algae) trap solar energy via photosynthesis and utilize the chemical reducing power to fix atmospheric nitrogen gas (N_2) to produce ammonia which then is utilized as the nitrogen source for cellular growth. The objective of this project is to understand the cellular differentiation processes which are required to allow N_2 fixation to proceed. The assimilation of N_2 and the incorporation of the reduced nitrogen into organic molecules occurs to specialize cells called heterocysts. These cells have been isolated and biochemically characterized. The following projects are currently being pursued in an effort to understand further the development of the specialized cells. Using recombinant-DNA technology we have constructed DNA clones designed to be capable of transfer to, and replication and selection in cyanobacterial cells, and to circumvent problems of genetic restriction. Such clones have been successfully transferred from Escherichia coli to, and replicated and selected in, unicellular as well as nitrogen-fixing filamentous cyanobacteria. With partial support from N.S.F., we are also constructing a physical-genetic map of the Anabaena genome using the cosmid cloning technique. Thus, we have made substantial progress toward developing tools for the genetic manipulation of photoautotrophic, nitrogen-fixing cyanobacteria. The significance of this work is that it opens the way to increased understanding of cellular differentiation and to construction of modified strains which would be particularly suitable for commercial application of biological solar energy conversion.

109. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ENVIRONMENTAL CONTROL OF PLANT DEVELOPMENT AND ITS RELATION TO PLANT HORMONES — $141,000
Jan A.D. Zeevaart, MSU-DOE Plant Research Laboratory

Environmental factors such as daylength, temperature and soil moisture content have pronounced effects on plant growth and development. Plant growth substances are often involved as intermediaries between the perception of an environmental factor and the ultimate morphological expression. The objectives of this program are to characterize the horsones involved, how their synthesis and catabolism are regulated by the environment, as well as to understand their mode of action. The following projects are currently under investigation.

a) Regulation of stem and leaf growth in the long-day rosette plant spinach by gibberellins (GAs). The aim is to determine how long days control the synthesis of the biologically active GA_{20} and how this in turn causes stem elongation.

b) Regulation of stem growth and flowering in dwarfed mutants of Arabidopsis thaliana and tomato which are deficient in gibberellins. The aim is to determine the steps at which the GA biosynthetic pathway is blocked in the various mutants.

c) Regulation of abscisic acid (ABA) synthesis, catabolism and compartmentation in response to water stress. Although ABA controls the loss of water by closing stomata, the bulk ABA in a leaf often does not correlate with stomatal aperture. The distribution of ABA at the organ, cellular, and subcellular level is therefore being studied in Xanthium strumarium and Vicia faba (supported in part by the National Science Foundation).

110. OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830

ENERGY AND NUTRIENT UTILIZATION EFFICIENCY IN INTENSIVE FOREST BIOMASS PRODUCTION: A STUDY OF SITE-SEEDLING INTERACTIONS — $200,000
S. B. McLaughlin, D. W. Johnson, N. T. Edwards, R. J. Luxmoore, R. F. Walker, Environmental Sciences Division

This study addresses plant physiological and soil-plant nutrient processes which are important considerations in the utilization of marginal land for silvicultural production of energy. The primary objective of this work is to provide physiological criteria for quantifying yield potential of biomass candidate species, to determine the role of soil-plant nutrient dynamics on productive potential of these species, and to provide important insights into the physiological basis of species' tolerance and adaptability to environmental stress. Four tree species, yellow poplar (Liriodendron tulipfera), loblolly pine (Pinus taeda), sweet gum (Liquidambar styriciflua) and black locust (Robinea pseudoacacia) are being studied in a 20 ha managed population. Treatments being examined include mycorrhizal preconditioning, variable rate and timing of nitrogen supply, and mulching. Plant physiological parameters being measured include whole tree allocation of energy between metabolic pools, plant water status, leaf photosynthetic rate, photosynthate allocation by foliage, and root and soil respiration rate. The kinetics of nitrogen mobilization, and movement through soil-plant nutrient cycles are being examined to quantify nutrient conservation mechanisms under varying rates of nutrient supply. These data will provide important insights into the interactions involved in seasonal allocation of carbon, water, and nutrients for representative biomass candidate species and aid in the selecting of criteria for enhancing biomass production potential.

111. SOLAR ENERGY RESEARCH INSTITUTE
Golden, Colorado 80401

BASIC PHOTOBIOLOGY RESEARCH $105,000

Paul F. Weaver, Stephen C.T. Lien, Michael Seibert
Photoconversion Research Branch

This work encompasses three areas of electron-transport studies associated with photobiological H_2 metabolism. Task 1 will determine the degree of integration among H_2 metabolism, N_2 fixation, photosynthesis, and the multiplicity of energy-conversion mechanisms present in photosynthetic bacteria, particularly Rhodopseudomonas and Rhodospirillum species. A broad spectrum of mutants is being generated with defective redox components operative in autotrophic or heterotrophic, anaerobic and aerobic, and light or dark growth modes. These defects are being characterized by pleiotrophic losses of other growth modes, spectral and enzymatic properties, and protein separation and quantitation techniques. The data will be used to amplify H_2 metabolism in organisms utilizing less energy intensive, ammonia-insensitive hydrogenase reaction rather than the nitrogenase pathway. Task 2 has led to the first purification of hydrogenase from a eucaryotic source (Chlamydomonas reinhardtii). Characterization of the physical, chemical and catalytic properties of the algal enzyme will be continued. The results obtained will be compared with those from procaryotic hydrogenases. In addition, special emphasis will be placed on developing a mechanistic model for the formation of a catalytically active complex between hydrogenase and various electron-mediators. Task 3 will investigate the water-splitting apparatus of oxygenic photosynthetic systems using biochemical techniques, electron microscopy and physical methods such as fluorescence induction, flash spectroscopy and direct, quantitative detection of O_2 yields. Chloroplasts and four types of O_2-evolving PS II preparations are being characterized by polypeptide-composition analysis, Mehler-reaction activities, EPR-detectable PS I, low-temperature fluorescence, steady-state and flash yields of O_2, and stability of O_2-production activity over extended time periods.

INDEX OF INVESTIGATORS
and Summary Number

Albersheim . . . 12
Armentrout . . . 28
Arntzen 99
Atalla 37
Bartholomew . . . 93
Bartsch 5
Bassham 94
Bauer 40
Beachy 71
Bearden 91
Bennett 85
Bogorad 26
Boyer 6
Breidenbach . . . 7
Bressan 61
Brill 78
Bryant 30
Burr, B. 86
Burr, F. 86
Burton 21
Canale-Parola . . 44
Carrico 52
Cashmore 63
Chelm 100
Cheniae 39
Chilton 72
Chollet 53
Clark 67
Clayton 13
Cleland 75
Conway de Macario 55
Cormier 19
Crawford 29
Crofts 31
Croteau 73
Darvill 12
Dutton 60
Ebrey 32
Edwards 110
Evans 40
Eveleigh . . . 64,65
Finnerty 20
Foard 62
Frea 58
Furlong 76
Gantt 66
Gardner 33
Gennis 34
Ghosh, A. . . . 65
Ghosh, B. . . . 65
Gibbs 4
Good 45
Hall 76
Handa 61
Hanna 21
Hanson, A. . . . 101
Hanson, R. . . . 46
Hasegawa 61
Hearst 95
Helentjaris . . . 61
Hind 87
Jenson 56
Johnson 110
Jones 8
Kamen 5
Kaplan 5
Kende 102
Kermicle 79
Key 22
King 61
Klein 96
Kleinhofs 74
Krulwich 51
LaRue 3
Lamport 103
Lancaster 70
Lang 104
Lanyi 9
Larkins 62
Laughnan 35
Lidstrom . . . 76,77
Lien 11
Ljungdahl 24
Long 68
Lurquin 74
Luxmoore 110
Macario 55
Madison 1
Mah 10
Mans 18
Matthews 15
McInerney 59
McIntosh 105
McLaughlin . . . 110
McNeil 12
Meagher 23
Mehlhorn 92
Messing 47
Montenecourt . 41,65
Nelson 80
O'Leary 81
Outlaw 17
Packer 9,92
Pearlstein . . . 2
Peck 24
Phillips 49
Poff 106
Pratt 25
Quail 82
Quintanilha . . . 92
Radmer 42
Rains 7
Rapoport 97
Reeve 58
Rogers 48
Rubenstein . . . 49
Salyers 33
Sands 41
Sauer 98
Saxton 7
Sciaky 88
Seibert 111
Sheir-Neiss . . . 65
Sherman 50
Siegelman 89
Smith 90
Somerville . . . 107
Stafford 57
Steponkus 14
Stewart 38
Sussman 83
Sze 43
Thompson 1
Tjepkema 27
Torrey 27
Ulrich 61
Valent 12
Van Etten 54
VanEtten 15
Walker 110
Weaver 111
Wills 11
Wolfe 36
Wolin 55
Wolk 108
Zeevaart 109
Zeiger 69
Zeikus 84
Zinder 16

L. BES Program Direction

1. **For the period FY 1981 - FY 1985, please provide actual and estimated operating expenses, as well as staffing levels for BES Program Direction.**

Answer:

	FY 1981 Actual	FY 1982 Actual	FY 1983 Actual	FY 1984 Estimate	FY 1985 Estimate
Operating Expenses (BA in thousands)	$2,500	$2,500	$3,170	$3,970	$3,830
Staffing (Full-time equivalents)	54	53	55	62	62

2. **The budget justification request (Congressional Budget Request, FY 1985, Volume 3, p. 175) states that BES program direction staff develops long-range plans. For the period FY 1981 - FY 1985, please list all completed, ongoing and planned long-range plans for BES.**

Answer: Long-range program planning documents developed under the BES program are normally working documents or reviews of selected scientific areas to identify research needs and the resources required to carry them out. BES technical staff direct or participate in such reviews, workshops, symposia or scientific planning activities making maximum use of relevant scientific expertise.

Procurement and financial management staff carry out required planning activities to identify commitment projections, especially with regard to major facilities and their effective utilization.

The following is a sample of the formal documents that have resulted from BES planning activities during the past five years. This list, while not complete, is indicative of the type of planning activities done on a regular basis.

1. BES INITIATIVE FY 1980-89: RADIOACTIVE WASTE DISPOSITION. September, 1979.

2. CONTINENTAL SCIENTIFIC DRILLING PROGRAM (NAS/NRC report). 1979.

3. THE ROLE OF FUNDAMENTAL BIOLOGICAL RESEARCH IN DEVELOPING FUTURE BIOMASS TECHNOLOGIES. Defines research priorities and identifies long-term research needs in the BES BIOLOGICAL ENERGY RESEARCH PROGRAM. Biomass 1 (1981) 17-37.

4. NAS/NRC Report. THE DEPARTMENT OF ENERGY: SOME ASPECTS OF BASIC RESEARCH IN THE CHEMICAL SCIENCES, PART 2. 1981.

5. NAS/NRC Report. SEPARATED ISOTOPES: VITAL TOOLS FOR SCIENCE AND MEDICINE. 1982.

6. DOE/ER-0172. Report on THERMOPHYSICAL PROPERTIES FOR SYNTHETIC FUELS, a survey in support of planning for the Engineering Research Program. August, 1983 (carried out in 1981 and 1982).

7. CONF-8209111. ENERGY MATERIALS COORDINATING COMMITTEE CONTRACTOR MEETING ON PROBLEMS AND OPPORTUNITIES IN STRUCTURAL CERAMICS. April, 1983.

8. NAS/NRC Report. OPPORTUNITIES AND CHALLENGES IN RESEARCH WITH TRANS-PLUTONIUM ELEMENTS. 1983.

9. LA-UR-83-1717. HEAVY ION ACCELERATOR RESEARCH PROGRAM PLAN FOR FY84-FY89. May, 1983.

10. CONF-830474. CRITICAL AND STRATEGIC MATERIALS: PROCEEDINGS OF THE LABORATORY STUDY GROUP MEETING. Focus on identifying and articulating high priority BES MATERIALS SCIENCES PROGRAM target areas. June 1983.

11. EGG-MS-6387. Report on WORKSHOP ON LONG RANGE PLANNING AND THRUST RESEARCH AREAS FOR THE DOE/BES ENGINEERING RESEARCH PROGRAM. August, 1983.

12. REPORT OF THE RESEARCH BRIEFING PANEL ON SELECTED OPPORTUNITIES IN CHEMISTRY. Research Briefings 1983, NAS. (Pimentel Committee - continuing).

13. NATIONAL ACADEMY OF SCIENCES PHYSICS SURVEY COMMITTEE - currently reviewing physics research.

14. NATIONAL ACADEMY OF SCIENCES MAJOR MATERIALS FACILITIES COMMITTEE - currently reviewing major facilities for materials research.

3. The budget justification (Congressional Budget Request, FY 1985, Volume 3, p. 175) notes that the Small Business Innovation Research (SBIR) Program awarded 106 contracts totalling over $5.0 million in FY 1983. Please provide a listing of these contractors, title of the proposals, and length and amount of the award.

Answer: Please See Attachments

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
Advanced Fuel Research, Inc.	On-Line Compositional Analysis of Solids by Photoacoustic FT-IR Spectroscopy	6	49,194
AGR, Inc.	The Strategic Importance of Detecting Subsurface Hydrocarbon-Bearing Astroblemes	6	39,600
Aleph Latoratories, Inc.	Research on Measuring Instrumentation for Cryogenic Systems	6	46,232
Altex Corporation	Extreme Ultraviolet and Soft X-Ray Instrumentation for Microcharacteri-zation of Materials	6	48,522

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
Analytics, Inc.	Development of an Eddy-Current Sensor and Algorithm for Three Dimensional Quantitative Nondestructive Evaluation	6	49,965
ANCO Engineers, Inc.	A Device for Failure Tolerant Transmission Line Design	6	44,428
Applied Coatings International, Inc.	Plasma Sprayed Wear-Resistant Self-Lubricating Coatings	6	49,775
Applied Microwave Plasma Concepts, Inc.	High-Beta Hot-Electron Surface-Layer Enhancement of Confinement in Stellarators	5	46,500
Atom Sciences, Inc.	Development of Sputter-Initiated Resonance Ionization Spectroscopy for Application in the Single-Atom Detection of Technetium	6	45,170
Bend Research, Inc.	Solvent-Swollen Membranes for the Removal of H_2S and CO_2 from Coal Gases	6	49,355
Bend Research, Inc.	Concentration of Synfuel Process Condensates by Reverse Osmosis	6	49,333
Bennett-Ringrose-Wolsfeld -Jarvis-Gardner, Inc.	Sunlight Distribution in Remote Interior Locations Using a Multi-Axis Suntracker as a Light Source	6	49,762
Cape Cod Research, Inc.	Chemical Separation of Dilute Wastes with Magnetic Absorbents	6	49,997
Carbotek, Inc.	Catalytic Cleanup of Lurgi and "In Situ" Raw Coal Gas	6	50,000
Castle Technology Corporation	Nickel and Cobalt Extraction from Laterites and Manganese Nodules	6	50,000
Cellulose Conversion Handbook Enterprises	Laser Tree Trimmer	6	19,500
Ceramic Finishing Company	Fracture Mechanics Investigation of Grinding of Ceramics	6	49,823
Ceres Corporation	Horizontal Growth of Silicon Sheet Crystals via Edge-Supported Pulling (ESP) from a Melt Contained in a Cold Crucible	6	50,000
Chemical and Metal Industries, Inc.	Recovery of Strategic Elements from Spent Petroleum Catalysts	6	48,108

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
Columbia Building Materials, Inc.	A Concrete Masonry Unit Building System for Passive Homes--Design, Manufacturing Feasibility, Construction Adaptability, and Thermal Properties Testing	5.5	46,729
Covalent Associates, Inc.	The Determination of Organic Acids in Fermentation Broths by an Electrochemical Sensor	6	49,611
Creare R&D, Inc.	Turboexpander for Cryogenic Helium Refrigerators and Liquifiers	6	47,062
Creare R&D, Inc.	High Speed Motor for Application in Miniature Gas Bearing Cryogenic Pumps	6	28,862
Crystal Systems, Inc.	Growth of Bismuth Germanate ($Bi_4Ge_3O_{12}$, BGO) Using the Heat Exchanger Method (HEM)	6	49,928
CVI Inc.	Closed Cycle Cryocooler with Hybrid Heat Exchanger-Regenerator	6	49,983
Dynamics Technology, Inc.	A SQUID-Based Airborne Magnetic Gradiometer System	6	48,598
Dynamics Technology, Inc.	Fiber Optic Particle Beam Monitor	6	48,409
EIC Laboratories, Inc.	Chemical Bath Deposition of $CuInSe_2$ for Solar Cells	6	49,970
EIC Laboratories, Inc.	Electrochromic Heat Mirrors for Photothermal Applications	6	49,432
EIKONIX Corporation	Digital Imaging Optical Extensometer	6	49,712
Electrochemical Technology Corporation	Mathematical Modeling of Stress Corrosion Cracking	6	43,249
ELTECH Systems Corporation	Catalyst for Electrochemical Ozone Generation	6	48,566
Eltron Research, Inc.	Birefringence Relaxation for Semiconductor Minority-Carrier Lifetime Measurement	6	48,898
Energetics, Inc.	Application of Artificial Intelligence to Process Control in the Pulp and Paper Industry	6	49,702
Environmental Protection Polymers, Inc.	Process for Disposal of Radioactive Waste	6	49,936
EXPORTech Company, Inc.	Magnetic Deashing of Coal	5.5	49,579

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
Facility & Manufacturing Automation, Inc.	Research and Development of Long-Life Cryogenic Seals	6	50,000
Fiber Materials, Inc.	High Performance Silicon Carbide and Silicon Nitride	6	47,680
Flow Industries, Inc.	Development of an Innovative Electrostatic Precipitator Design	6	49,210
Foster-Miller, Inc.	Generation and Use of Dirty Steam from Wastewaters in Coal Conversion Plants	6	45,360
Foster-Miller, Inc.	Heavy Fluid Beneficiation Centrifuge	6	48,510
Genetics International, Inc.	Hydrogen Peroxide Monitor	6	48,285
GINER, Inc.	Electrochemical Hydrogen Separation	6	49,792
Greenbriar Systems, Inc.	Automation of the Detection of Defects in the Heat-Exchanger Tubing of Nuclear Steam Generators	6	49,004
Gumbs Associates, Inc.	Polymer Laminates for Solar Energy Applications	6	48,033
Helipump Corporation	Modelling and Simulation of Electrolytic Cells	6	46,969
Helipump Corporation	Antisolvent Extraction of Lignin	6	49,798
Helix Associates, Inc.	Process for the Manufacture of 2,2',4,4' Tetrahydroxybenzophenone	6	45,000
HPM Corporation	Method for Heatless Production of Foundry Shell Molds	5.5	46,850
ICR Research Associates, Inc.	Fourier Transform Mass Spectrometer for Analysis of Complex Fuel Mixtures	6	49,275
INET Corporation	Feasibility of Digital Signal Conditioning for Test Instrumentation Using Large-Scale Integrated Circuits	6	49,172
Inference Corporation	Adding Heuristic Knowledge to Computer Algebra Systems	6	47,995
Intermountain Technologies, Inc.	Application of Fluid Bearings to Turbine Flow Meters	4.5	43,114

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
KLM Engineering, Inc.	Development and Fabrication of a Prototype Fiberglass Container for Transporting and Storage of DOT Type A Radioactive Waste	4.5	48,142
KLM Engineering, Inc.	Development of a Gas Permeable Membrane System for Radioactive Gas Processing	5	47,950
KMS Fusion, Inc.	Theoretical Research on the Evaporation of Pellets in Tokamak Plasmas	6	49,940
KSE, Inc.	Stability and Compatibility of Heavy Oil Conversion Product Blends	6	45,379
Lehrer-Pearson, Inc.	Defining Electron Beam Quality in Terms of Electrode Form and Position Precision	9	48,569
Magna-Power Electronics	Phase Modulated Photovoltaic Inverter	6	43,400
Management and Technical Consultants, Inc.	Investigation of an Advanced Concept for the Reforming of Heavy Liquid Hydrocarbon Fuels to Hydrogen	6	50,000
Materials Engineering Associates (CA), Ltd.	High Temperature and/or High Speed Thickness Gauging of Metals	6	43,535
Maxwell Laboratories, Inc.	Impurity Transport Diagnostic Development for Magnetically Confined Fusion	6	48,646
McIver Consultants International	Wide-Range Downhole Flowmeter Logging Tool	6	49,911
Measurement Concepts, Inc.	Development of a Single Aperture-Four Channel Nanosecond Polarimeter for Application to the Non-Destructive Evaluation of Materials	6	37,703
Membrane Technology and Research, Inc.	A Novel Liquid Ion Exchange Extraction Process	6	50,000
Mertz, Inc.	Feasibility Investigation of an Air Transportable Seismic Vibrator	6	50,000
Mission Research Corporation	Numerical Simulation Study of the Plasma Beatwave Accelerator Concept	6	49,738
MMP Technologies, Inc.	Microminiature Refrigerators for Cooling Instrumentation in Downhole Logging	6	50,000
National Electrostatics Corporation	Design of Components for an Ampere Intensity, MeV Energy, DC Electron Beam System	4	25,150

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
Nuclear Data, Inc.	Primary Coolant Radionuclide Characterization, Modelling, and Reduction	6	49,963
NYCB Real-Time Computing, Inc.	Development of a 32-Bit Single Board Computer System in FASTBUS Packaging	6	49,183
OMEGA-P, Inc.	Wiggler-Free Free Electron Laser for Plasma Heating	5	49,949
Ophir Corporation	An Infrared Absorption Hygrometer for Use in Primary Coolant Loops of Gas-Cooled Nuclear Reactors	6	48,693
OPTIMA Systems, Inc.	A High Speed Optical Pressure Sensor for Cylinder Pressure Measurement of Internal Combustion Engines	6	49,735
OPTRA, Inc.	Fiber Optic Current Probe	6	42,415
OWNET, Inc.	Nondestructive Detection Device for the Radiation Damage in Nuclear Pressure Vessels	6	49,443
Phase Change Technology, Inc.	Development of Building Components Containing Advanced Phase Change Materials	6	49,941
Plant Resources Institute	Supercritical Fluids and Azeotropic Solvent Systems as Alternatives to Conventional Solvent Extraction of Biomass	6	49,986
Radiation Monitoring Devices, Inc.	Solid State Nuclear Sensors for High Temperature Oil Well Logging	6	50,000
Radiation Monitoring Devices, Inc.	Avalanche Photodiodes for Positron Emission Tomography	6	50,000
Rasor Associates, Inc.	Cesium Dispensing Negative Ion Formation Electrodes	6	49,654
Resource Engineering, Inc.	Apparatus for Fine Coal Cleaning	6	49,495
Reuter-Stokes, Inc.	Design of a Long, High-Sensitivity Fission Counter	6	37,703
Scientific Measurement Systems, Inc.	Uranium Fuel Rod Inspection by High Resolution Tomography	6	49,596

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
Scientific Systems International	FASTBUS Segment Extension as a Crate Coupling Technique	6	19,353
Sea Data Corporation	Fast Response Hydrodynamic Oxygen Probe for Bioreactors	6	48,783
Soil and Land Use Technology, Inc.	Increased Production of Extractives in Woody Plants	6	49,799
Southwest Research and Development Company	Optical Strain Measurement Device	6	38,600
Spectral Sciences, Inc.	Spark Discharge Moisture Monitor	6	50,000
Spectral Sciences, Inc.	Infrared Moisture Monitor	6	50,000
Spectron Development Laboratories, Inc.	Design of a Multi-Element Programmable Fuel Nozzle for Effective Atomization of Liquid and Slurry Fuels Under Variable Load Conditions	6	49,953
Spectron Development Laboratories, Inc.	Stepped Frequency Ultrasonic Holography for Flaw Characterization	6	46,490
Spire Corporation	Single-Crystal Silicon Films for Limit-Efficiency Solar Cell Structures by 3-Dimensional Graphoepitaxy on Metal Mirrors	6	48,247
Spire Corporation	Feasibility of Advanced Cell Designs for High Efficiency Flat-Plate Applications	6	48,189
Supercon, Inc.	An Investigation to Determine the Commercial Feasibility of "In Situ" Copper-Niobium Composites for High-Strength, High-Conductivity Applications	6	49,966
Synergetics, Inc.	Variable-Area, Light-Reflecting Assembly (VALRA)	6	49,786
Technology for Energy Corporation	A High-Speed, Curved, Position-Sensitive X-Ray Detector	6	41,364
TERA Advanced Services Corporation	Evaluating the Chemical Recycling Plant for the Oxygen-Iodine Photodetachment Laser	5	49,899
The Arizona Carbon Foil Company, Inc.	Improving Carbon Foils	6	49,516
TOFTEC	High Resolution Time-of-Flight Mass Spectrometer	6	34,939

Contractor	Proposal Title	Length of Award (Mos.)	Amount of Award ($)
UNIVERSAL ENERGY SYSTEMS, Inc.	Fabrication of Amorphous Metallic Films and Coatings for Industrial Applications Using High Energy Ion Beam Mixing	6	49,943
UNIVERSAL ENERGY SYSTEMS, Inc.	Development of Hot Corrosion-Resistant Alloys Using Ion Beam Processing	6	49,990
Viking Energy Corporation	Identification of Potential Robotic Applications in the Management of Radioactive Wastes at the West Valley Demonstration Project	6	49,775
Viking Instruments Corporation	Development of a Field-Portable GCMS for Analysis of Hazardous Energy-Related Substances	6	48,987
Virginia Transformer Corporation	Solid State, On Load Tap Changer for Power Transformers	6	41,321
Western Research Corporation	Photocathode Production of High Power RF	6	48,359

4. **What level of funding will be available for the SBIR Program in each of FY 1984 and FY 1985, and how many awards are expected to be made for each of these two fiscal years?**

   Answer: Funding levels of $15.8 million and about $26.1 million will be available for the SBIR Program in FY 1984 and FY 1985, respectively.

   In FY 1984 the Program will make approximately 100 Phase I awards, totalling about $5.0 million, and approximately 50 Phase II awards. Only the first year of the Phase II contracts - typically 2 years in duration - will be supported out of FY 1984 funds, at a total cost of about $10.8 million.

   In FY 1985, about $10.5 million will be spent to continue the Phase II contracts, initiated the previous year, into their second year. Also, approximately 100 new Phase I awards and approximately 50 new Phase II awards will be made. The total value of the Phase I awards will be about $5.0 million; only the first year of the new Phase II contracts will be supported out of FY 1985 funds, at a total cost of about $10.6 million.

5. **What were the program "taxes" levied to support the SBIR Program in FY 1983, and what "taxes" are expected in FY 1984 and FY 1985?**

   Answer: SBIR Program support has been allocated within the Department to each of the Assistant Secretaries. This support for FY 1983, FY 1984, and FY 1985 is detailed in the table below (B/A in Thousands):

	FY 1983	FY 1984	FY 1985
Nuclear Energy	$ 1.6	$ 4.0	$ 6.0
Energy Research	2.4	8.0	14.7
Conservation and Renewable Energy	0.6	2.1	3.3
Fossil Energy	0.4	1.6	2.0
Radioactive Waste	0	0.1	0.1
Total	$ 5.0	$ 15.8	$ 26.1

6. **What criteria are used to judge the quality of a SBIR proposal? What sort of "scoring" system is used?**

Answer: The criteria used in judging the quality of a SBIR proposal, depending on whether it is for Phase I or Phase II of the program, follow below. Phase I criteria:

1. The scientific/technical quality of the Phase I research proposal and its relevance to the proposal's stated objectives, with special emphasis on its innovation and originality.

2. Qualifications of the principal investigator, other key staff, and consultants, if any, and the adequacy of available or obtainable instrumentation and facilities.

3. Anticipated benefits, technical and/or economic, of the proposed research (Phase I and Phase II), if successful.

4. Adequacy of the Phase I proposed effort to show progress toward proving the feasibility of the concept.

Phase II criteria:

1. The scientific/technical quality of the proposed research, with special emphasis on its innovation and originality.

2. The qualifications of the principal investigator and other key personnel to carry out the proposed work.

3. Anticipated benefits, technical and/or economic, of the proposed research.

4. Degree to which the Phase I objectives were met at the time of Phase II proposal submission.

5. The adequacy of the Phase II objects to meet the problem or opportunity.

A proposal is scored against the above criteria, as appropriate for either Phase I or Phase II, with approximately equal consideration being given to each criterion, except for an assignment of double weight to the first criterion listed for either case.

7. **How does the DOE plan to assess the effectiveness of the SBIR Program? What measures of effectiveness/performance will be used?**

Answer: The plan for assessing the DOE experience with SBIR is focused on the analysis of program results relating directly to the specific purposes of P.L. 97-219, as stated under Section 2(b) of this amended Small Business Act: (1) to stimulate technological innovation; (2) to use small business to meet Federal research and development needs; (3) to foster and encourage participation by minority and disadvantaged persons in technological innovation; and (4) to increase private sector commercialization innovations derived from Federal research and development. The analysis will also examine distinctions from non-SBIR programs within DOE, with a view towards determining if SBIR fills a special niche, playing a distinctively beneficial role, in the overall DOE R&D program. Data for this assessment will be drawn from the SBIR office files, from the participating technical programs within DOE, and from funded projects in the small business community.

M. BES Construction

1.0 Project 84-ER-141, General Plant Projects

1. **The construction project data sheets for GPP accompanying the FY 1984 budget request indicated that the GPP request of $400,000 would be used at Ames Laboratory ($275,000); at Notre Dame Radiation Laboratory ($25,000) for "minor building modifications to properly house staff members and to make optimum use of laboratory research space"; and at the Sandia National Laboratories' Combustion Research Facility for the "conversion of light duty work space to heavy duty laboratory space." What will be the actual distribution of the FY 1984 GPP funds, and what are the reasons for any changes?**

   Answer: FY 1984 GPP funds have been distributed in the same amounts as presented in the Congressional data sheet. Ames Laboratory has received $275,000, Notre Dame has received $25,000, and Sandia National Laboratory has received $100,000.

2.0 Project 85-ER-400, General Plant Projects

2. **The FY 1985 Notre Dame Radiation Laboratory GPP request includes $50,000 for "minor building modifications to properly house staff members and to make optimum use of laboratory research space." Why are these funds requested when a similar request was included in the FY 1984 request?**

   Answer: Experience within the Department indicates that minor new construction and minor alterations to buildings and utility systems are required on an annual basis to conduct an effective and efficient research program. The request for Notre Dame is no exception. The $50,000 request for Notre Dame in our view is a sound investment given the capital base which exists at the university and the size of the research program being undertaken.

3. **What are the reasons that Argonne's GPP funding is now included here?**

   Answer: It has been the practice of the DOE to assign GPP and GPE funding responsibility for a given laboratory to the program providing the greatest amount of support to that laboratory. In FY 1984 and prior years, the Assistant Secretary for Nuclear Energy's (NE) Breeder Program budgeted these funds for ANL. An analysis of funding trends to ANL prior to the submission of the FY 1983 budget showed declining Breeder Program support to ANL, most of which went to ANL-West, and that the Office of Energy Research's Basic Energy Sciences Program was increasing its support of ANL activities. Thus, the decision was made to transfer funding responsibility to the BES program in 1985.

3.0 Project 84-ER-141, Accelerator Improvements and Modifications

4. The FY 1984 budget request of $1.26 million included $140,000 for the High Flux Beam Reactor and $500,000 for the NSLS at Brookhaven; $100,000 for the Dynamitron at Argonne; and $250,000 for the En-Tandem and $270,000 for the Calutrons at Oak Ridge. What will be the actual distribution of these funds in FY 1984, and what are the reasons for any changes?

Answer: A small reallocation of funds has been made involving two of the projects prepared in the FY 1984 budget. This redistribution involves the NSLS project and the HFBR project. In FY 1984 we now plan to fund $600,000 for NSLS and $40,000 for HFBR. The successful commissioning of the X-ray ring and upgrading of the VUV ring has been assigned a high priority. This fact, coupled with the assignment of a lower priority to originally planned projects for the HFBR, (without adverse effect on reactor safety or operational efficiency) led to the decision. The other projects remain unchanged.

Projects planned for NSLS include: improvements to the vacuum systems, improved LINAC performance, and projects for the elimination of instabilities in the VUV ring. The HFBR projects to be deferred include replacement of control room recorders and replacement of the Cold Neutron Facility turbines. Both of these projects will be completed in FY 1985.

4.0 Project 85-ER-401, Accelerator Improvements and Modifications

5. What is the Bulk Shielding Reactor at Oak Ridge National Laboratory?

Answer: The Bulk Shielding Reactor is a 2 MW light water reactor with a movable core in a swimming pool-type container. It is being improved to accommodate a cryogenic temperature neutron irradiation facility with the highest neutron flux at the temperature of 4°K in the United States, and will be a national user facility open to qualified researchers. Some of the research to be performed will be studies of ductile-brittle transitions in steels, neutron irradiation effects at cryogenic temperatures of superconductors and magnets, and studies by electron microscopy at 4°K of neutron irradiation induced defects at cryogenic temperatures in materials and in biological specimens.

5.0 Project 85-ER-402, Stanford Synchrotron Radiation Laboratory Enhancement

6. What is the date of the last cost estimate for this project?

Answer: The latest cost estimate was submitted on August 26, 1983, and is $12,930,000 as reflected in the FY 1985 Congressional budget.

7. Is the cost estimate of $12.93 million in FY 1984 dollars, in FY 1985 dollars, or in as-year spent dollars? What escalation rates are assumed for the project?

Answer: The cost estimate was calculated on the basis of as-year spent funds. Escalation rates for the years 1983-1984 were 8.0%, 1984-1985 at 8.5% and 1985-1986 at 9.0%.

6.0 Project 85-ER-403, Ion Collision Physics Facility, Kansas State University

8. When was the last cost estimate for the project?

Answer: The last cost estimate for this project was made in September 1983.

9. Is the cost estimate of $3.4 million in FY 1984 dollars, in FY 1985 dollars, or in as-year spent dollars? What escalation rates were assumed in this estimate?

Answer: The cost estimate of $3,400,000 is in as-year spent dollars. An escalation rate of 8% has been assumed to the mid-point of construction.

10. How does this university rank in the nation with respect to the quality of graduate programs in atomic physics? Please provide documentation.

Answer: This type of data is not available as such. What is available are peer reviews from 6 scientists obtained in 1982 that are relevant to this inquiry. The reviews are attached and indicate the value of the KSU research in atomic physics relative to the rest of the country and the world.

Excerpts from these reviews and pertinent to this question are as follows. (The Roman numeral indexes the specific review found in the attachment.)

Review I:

The KSU program has grown into and remains the strongest university-based accelerator program dedicated almost exclusively to atomic collision physics. A modest nuclear physics component survives but is not substantial enough to stand on its own. In spite of the tragic loss, a few years ago, of one of its most talented and imaginative staff members, the KSU program has retained or regained its vitality. Its geographic remoteness notwithstanding, KSU is on the itinerary of virtually every international atomic collision physicist visiting this country. Recently, the laboratory has made great strides by pursuing a new initiative on the production by recoil and the subsequent experimental use for capture measurements of low-velocity highly-charged ions. Certainly, the proposal conveys the impression that the KSU group is taking advantage of new opportunities and not just resting on its laurels.

Review II:

Overall, I think this proposal should be supported. It is probably the best University program of research in atomic collisions of ions of both high and low velocity. The only comparable work in this field comes from Tokyo, Aarhus and Darmstadt, where there is strong support for such accelerator programs. The KSU work is as far ahead as any of these other groups, and especially in the recoil ion work has the best program.

Review III:

The Kansas group has made some of the most significant advances in the study of the production and use of highly stripped, low-velocity recoil ions.

The Kansas group is the most active and productive group in accelerator based atomic physics in this country. Its proposed budget is reasonable in relation to the size of its group and its program. The group deserves full DOE support.

Review IV:

The experiments proposed in this section (A. High-Velocity, Highly-Charged Ions) are, for the most part, extensions of an experimental program which has over the years, provided a wealth of high quality data on ionization, electron capture, and decay systematics of heavy-ions at high velocity. In this area, the Kansas State group has attracted widespread international recognition and their work is unsurpassed anywhere in the world.

Review V:

The group at KSU has done, and if this proposal is any indication, will do the best work in atomic collision physics in the United States. The basic staff, Richard, Cocke, Gray, McGuire, Hagmann and Lin are all excellent scientists. In addition, KSU has been able to attract top quality scientists and post-docs from abroad and the U.S. to collaborate with their experiments.

I urge that the DOE give this laboratory its utmost support in the next three years.

Review VI:

It is my judgment that the research proposed here is worthy of continued support based on its basic scientific merit, the qualifications of the research staff, the quality of the accelerator facility, and the relevance of much of the work to the perceived interests of DOE. I recommend that the proposal be funded at an appropriate budget level.

11. How many graduate degrees have been awarded from this institution over the past ten years? How does Kansas State University rank in quantity produced compared with other universities which award graduate degrees in atomic physics?

Answer: The following table shows the number of graduate degrees granted by Kansas State University during 1974 - 1983:

Graduate Degrees Granted by Kansas State University

Year	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983
# Degrees	830	794	849	997	971	846	863	842	878	787

Comparative data on graduate degrees in atomic physics are not available. Doctorate degrees granted in the combined disciplines of atomic and molecular physics are available but are not directly comparable to the graduate degrees in atomic physics granted by Kansas State University. With that reservation the following data is presented:

Graduate Degrees Granted by Kansas State in Atomic Physics

Year	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983
Numbers	2	8	2	4	2	1	5	3	1	6

PhD Degrees Granted by all U. S. Universities in Atomic and Molecular Physics

Year	1974	1975	1976	1977	1978	1979	1980	1981	1982
Number	120	138	116	106	88	72	69	65	96

The only record accessible shows that in 1982, 148 institutions reported granting doctorates in physics and astronomy. The figure of 148 is an upper limit in determining an institutional average of PhD degrees granted in physics. Kansas State granted 6 PhD degrees in Physics in 1982, one of which was in atomic physics as indicated in the table above. The six degrees granted by Kansas State are far above the national average for 1982, viz., 96/148 or less than one PhD degree per institution.

7.0 Project 84-ER-111, Beam Lines and Support Area Construction, NSLS

12. Were the project's February 1982 and September 1983 cost estimates of $19,700,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: Both estimates were in as-year spent dollars.

13. What escalation rates were assumed in the February 1982 estimate? How have the actual escalation rates compared with the February 1982 estimate?

Answer: The February 1983 estimate assumed 9.3%, 9.1%, and 8.4% for FY 1983 through FY 1985. This is noted in section 10 footnote 2 of the data sheet. Insufficient procurement activity has occurred to date to allow proper assessment of actual escalation rates on the project. The only significant experience was obtained with the AE contract which required extensive negotiation and a slight deferral of services to comply with the budgeted funds.

14. What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the February 1982 estimate?

Answer: There has been insufficient construction experience to date to allow for the development of specific project escalation rates. There have been no shortages or overages detected at this time.

15. What changes in the project's scope were made between the February 1982 estimate and the September 1983 estimate?

Answer: No significant changes in the project's scope on conventional construction were made between the February 1982 estimate and the September 1983 estimate. However, rapidly changing progress in the state-of-the-art of insertion devices, and beam line fixtures has resulted in changes in the numbers and characteristics of these components. Such variations were forecast in both the February 1982 and September 1983 proposals. Moreover it is likely that further state-of-the-art changes and new research requirements will occur over the scheduled construction time period in the rapidly advancing field of synchrotron radiation beam lines and insertion devices.

16. How much of the project's $2,595,000 contingency remains?

Answer: In these early stages of the project no contingency funds have been firmly allocated to the various work breakdown section elements. However, it is anticipated that about $250,000 of these funds will soon be allocated to expected A/E costs and beam line design costs in the second half of FY 1984.

II. ENERGY RESEARCH ANALYSIS

1. **What has been and will be the level of funding for the Energy Research Analysis Program for the period FY 1981 - FY 1985?**

   Answer: Funding provided and expected is as follows:

Budget Authority (In Millions)				
FY 81	FY 82	FY 83	FY 84	FY 85
$12.5*	$2.983	$2.819	$2.869	$3.0

   * In 1981, the program included funding for Advanced Technology Projects and Satellite Power System. These programs subsequently were terminated. The Office of Program Analysis' Budget Authority was $2.5 million.

2. **For the period FY 1981 - FY 1985, please provide a listing of technical and program assessments planned and completed by the Energy Research Analysis Program, and the cost and performer of each.**

   Answer: See Attachment 1.

ATTACHMENT 1

OFFICE OF PROGRAM ANALYSIS (OPA)
PROGRAM AND TECHNICAL ASSESSMENTS
($ IN THOUSANDS)

FY 1981 Obligations

A. Program Assessments

- Assessment of the Office of Health and Environmental Research Program (OPA Staff) (1)..... $ 551
- Topical Reviews: The Physics and Chemistry of Acid Precipitation; Assessment of Some Energy Technologies Associated with Solar Energy; Climatic Effects of Minor Atmospheric Constituents (SRI-JASON)..... $ 200
- Review of the Advanced Technology Projects for Continuation (OPA Staff)..... 0
- Review of MHD Planned Program (OPA Staff)..... 0

B. Technical Assessments

- Technology Base Review, DOE R&D Programs (OPA) Staff..... $ 595

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(1) In each case that OPA Staff is listed, this staff is directly responsible for preparing a technical report; but, typically, Oak Ridge National Laboratory, Los Alamos National Laboratory, or other technical support may have been contracted for assistance.

- R&D Needs in Coal Liquefaction (University of California/San Diego, Fossil Energy Research Working Group)..... $ 70
- Research Needs in Coal Utilization and Synthetic Fuels Production (American Physical Society)..... $ 10
- Assessment of Factors Affecting Potential of Ethanol as a Transportation Fuel (OPA Staff)..... $ 20
- Assessment of Biomass and Algae (Ecoenergetics, Inc.)..... $ 30
- Assessment of Shale Beneficiation (Massachusetts Institute of Technology)..... $ 88
- Review of Foreign Technology Photosynthetic Production of Fuels and Chemicals (Lawrence Livermore National Laboratory)..... $ 45
- Review of Acid Rain Research (West Point Military Academy)..... $ 15
- Assessment of Liquid Air Engines (R&D Associates)..... $ 100
- Future Availability of Catalyst Metals (Midwest Research)..... $ 54
- Food Chain/Energy Studies (Washington University/St. Louis)..... $ 129
- Energy Research Advisory Board (Los Alamos National Laboratory and Koba Associates)..... $ 590

Total FY 1981 Obligations..... $2,497

FY 1982 Obligations:

A. Program Assessments

- Peer Review and Assessment, Basic Energy Science Program (OPA Staff)..... $ 355
- Assessment of Adequacy of Energy Research Reactor Safety Activities (OPA Staff)..... $ 0
- Seminar on Acid Precipitation (General Research Corporation).... $ 14
- Assessment of Electrochemical Storage Program (OPA Staff)..... $ 0
- Review and Coordination of Review Comments, Draft National Acid Precipitation Assessment Plan (OPA Staff)..... $ 0
- Research Needs Methodology/Procurement Study (OPA Staff)..... $ 5
- Assessments of the Office of Health and Environmental Research's Accomplishments (OPA Staff)..... $ 310
- Interagency Task Force on Acid Precipitation (National Laboratory Consortium)..... $ 25

- An Operational Research Plan for Acid Precipitation (National Laboratory Consortium)..... $ 200

B. Technical Assessments

- Assessment of Research Needs in Energy Conversion and Conservation (Research and Management Technicians, Inc.)..... $ 100
- Assessment of the Office of Health and Environmental Research's Nuclear Instrumentation Accomplishments (Ecosometrics, Inc.).... $ 58
- Assessment of the Office of Health and Environmental Research's Environmental and Health Indentification and Evaluation Accomplishments (SRA Corporation)..... $ 60
- Assessment of Research Needs for Geothermal Energy (Engineering and Economics Research)..... $ 50
- Review and Commentary on Paper Drafted by the United States/Canada Coordinating Committee on Transboundary Air Pollution (OPA Staff)..... $ 0
- Assessment of Research Needs in Nuclear Waste (Southern Science Applications, Inc.)..... $ 100
- Topical Reviews: Heavy Ion Fusion; Overview of the Physical-Chemical Processes in the Formation of Acid Precipitation; CO_2 and Climate; Production of Nuclear Material (JASON)..... $ 200
- Assessment of Research Needs in Solar Thermal (TPI, Inc.)..... $ 74
- Methanol and Ethanol as Alternative Fuels for Automotive Piston Engines (OPA Staff)..... $ 0
- Assessment of Research Needs in Photovoltaics (DHR, Inc.)..... $ 86
- Assessment of Coal Combustion (Coal Combustion Applications Working Group, University of California)..... $ 88
- Acid Precipitation Research Assessment Support (West Point Military Academy)..... $ 50
- Technology Base Assessments, DOE R&D Programs (OPA Staff)..... $ 428
- Assessment of Research Needs in Drilling and Other Assessment Assistance (Oak Ridge National Laboratory and Sandia National Laboratories)..... $ 75
- Energy Research Advisory Board (Oak Ridge National Laboratory and Koba Associates)..... $ 685

Total FY 1982 Obligations..... $2,963

FY 1983 Obligations

A. Program Assessments

- Assessment of Major Accomplishments of the Office of Health and Environmental Research (OPA Staff)..... $ 75
- Preparation and Coordination of Input to Annual Science and Technology Report to Congress (OPA Staff)..... $ 0
- Interagency Task Force on Acid Precipitation (OPA Staff)..... $ 44
- Preparation and Coordination of Executive Summary and Other Parts of the Interagency Task Force on Acid Precipitation's Annual Report (OPA Staff)..... $ 0
- Commentary on "National Strategy for Fast Breeder Reactor Development" (OPA Staff)..... $ 0
- DOE Input to the International Energy Agency's Annual Report on Energy R&D (OPA Staff)..... $ 0
- International Energy Agency's Energy Technology Studies (Brookhaven National Laboratory)..... $ 12
- Peer Review and Assessment of Research Programs in Enhanced Oil and Gas Recovery (OPA Staff)..... $ 165
- Assessment of DOE Position on Private Ownership of Civil Land Remote Systems (OPA Staff)..... $ 0
- Peer Review and Assessment of Solar Research Projects at the National Bureau of Standards (OPA Staff)..... $ 60
- Peer Review and Assessment of Conservation Projects at the National Bureau of Standards (OPA Staff)..... $ 0
- Assessment of Report by Donald Rice, Rand Corporation, on Need for Clinch River Breeder Reactor (OPA Staff)..... $ 0

B. Technical Assessments

- Interagency Memorandum of Understanding with the Environmental Protection Agency on Acid Precipitation (Brookhaven National Laboratory)..... $ 520
- Acid Precipitation Research Assessment Support (West Point Military Academy)..... $ 15
- Battery Technology Transfer (Argonne National Laboratory)..... $ 125
- Risk Analysis - Atmospheric Dispersion from Acid Rain (Brookhaven National Laboratory)..... $ 80

- Risk Analysis - Liquid Metal Fast Breeder Reactor (Oak Ridge National Laboratory)..... $ 125
- Acid Rain Transport Experiment Support Proposed by the Tennessee Valley Authority (Oak Ridge National Laboratory)..... $ 23
- Drilling Research Assessment (Oak Ridge National Laboratory and Sandia National Laboratories)..... $ 52
- Modeling Symposium - Acid Rain (Oak Ridge National Laboratory).. $ 50
- Assessment of Coal Combustion Long-Range Research (Coal Combustion Applications Working Group, University of California)..... $ 11
- Topical Reviews: Acid Rain; Tailored Nuclear Weapons; Photovoltaics; Muon Catalyzed Fusion (JASON)..... $ 200
- Assessment of Research Needs in Photovoltaics (DHR, Inc.)..... $ 27
- Assessment of Research Needs in Energy Conversion and Conservation (Research and Management Technicians, Inc.)..... $ 10
- Assessment of Current Status and the Potential of Alternate Power Reactor Concepts (OPA Staff)..... $ 0
- Reviews of Technology Development Histories for the International Energy Agency's Energy Technology Policy Study (OPA Staff)..... $ 0
- Reviews of Foreign Technology (Foreign Applied Sciences Assessment Center)..... $ 140
- Energy Research Advisory Board (Oak Ridge National Laboratory and Koba Associates)..... $ 613
- Assessment of Needs in Continental Scientific Drilling (Columbia University)..... $ 98
- Assessment of Factors Influencing Public Perceptions of Energy Systems Deployment (DuPont Associates)..... $ 87
- Acid Rain Research and Other Assessment Support to OPA Staff (Oak Ridge National Laboratory)..... $ 287

Total FY 1983 Obligations..... $2,819

FY 1984 and FY 1985 Estimates:

A. Program Assessments

- Assessment of Extent to Which Research Recommendations of Prior Review Panels in Fossil Energy Have Been Carried Out (OPA and Fossil Energy Staff)..... $ 0

- Assessment of Need for Continuation of High Altitude Sampling Program in the Office of Health and Environmental Research (OPA Staff)..... $ 0

- Peer Review and Assessment of the Advanced Research and Technology Development Projects in Fossil Energy (OPA Staff).... $ 400

B. Technical Assessments

- Assessment of Research Needs in Drilling (Oak Ridge National Laboratory and Sandia National Laboratories)..... $ 64

- Atmospheric Studies and Other Research Needs (JASON)..... $ 400

- Assessment of Four Solar Technologies for H_2 Production (Solar Energy Research Institute)..... $ 100

- Assessment of Research Needs in Large-Scale Systems (Carnegie-Mellon University)..... $ 53

- Assessment of Fuel Cell Research (University of California, Advanced Fuel Cell Working Group)..... $ 129

- Reviews of Foreign Technology (Foreign Applied Sciences Assessment Center)..... $ 280

- Assessment of Research Needs in Acid Precipitation (Brookhaven National Laboratory, Oak Ridge National Laboratory and Pacific Northwest Laboratory)..... $1,047

- Support of Interagency Task Force on Acid Rain (OPA Staff)..... $ 87

- Assessment of Technology Status: International Energy Agency (Department of Energy, International Energy Agency, and Brookhaven National Laboratory)..... $ 52

- Assessment of Bioengineering and Bioconversion Energy Research Needs (Under Request for Proposals)..... $ 125

- Assessment of Wind Energy Research Needs (Under Request for Proposals)..... $ 125

- Assessment of Nonhighway Transportation Research Needs (Under Request for Proposals)..... $ 125

- Assessment of Materials Research Needs for Advanced Energy Technologies (Under Request for Proposals)..... $ 125

- Interagency Memorandum of Understanding with the Environmental Protection Agency on Acid Precipitation (Oak Ridge National Laboratory)..... $ 240

- Improved PWR Fuel (OPA Staff)..... $ 6

- Program and Technical Assessment Support (National Laboratories and Others)..... $1,311
- Energy Research Advisory Board (Oak Ridge National Laboratory and Others)..... $1,200

Total FY 1984 and FY 1985 Estimated Obligations..... $5,869

3. **Please provide a listing of all DOE advisory committees and the current membership of each.**

Answer: Attachment A is a list of all Advisory Committees. Attachment B is a list of the membership of all Advisory Committees.

Attachment A

DEPARTMENT OF ENERGY ADVISORY COMMITTEES

1. ADVISORY COMMITTEE ON FEDERAL ASSISTANCE FOR ALTERNATIVE FUEL DEMONSTRATION FACILITIES (established by Public Law 93-577, as amended by Public Law 95-238)

   Objectives: To provide advice to the Secretary of Energy on matters relating to the development of alternative fuels.

2. ADVISORY PANEL ON ALTERNATIVE MEANS OF FINANCING AND MANAGING RADIOACTIVE WASTE FACILITIES

   Objectives: To study and report to the Department of Energy on alternative approaches to managing the construction and operation of civilian radioactive waste facilities, pursuant to Section 303 of the Nuclear Waste Policy Act of 1982 (Public Law 97-425). The Panel's report will include a thorough and objective analysis of the advantages and disadvantages of each alternative approach. The Panel shall complete and deliver its report to the Department by October 15, 1984.

3. AMERICAN STATISTICAL ASSOCIATION COMMITTEE ON ENERGY STATISTICS

   Objectives: Provide recommendations based on reviews of elements of Energy Information Administration (EIA) information collection and analysis programs; advice on priorities of technical and methodological issues in the planning, operation, and review of EIA statistical programs; and advice on matters concerning improved energy modeling and forecasting tools, particularly regarding their functioning, relevancy and results.

4. DOSE ASSESSMENT ADVISORY GROUP

   Objectives: To provide the Secretary of Energy and the Manager, Nevada Operations Office (NV), with advice and recommendations pertaining to the Offsite Radiation Exposure Review project. This project concerns the evaluation and assessment of the amount of radiation received by members of the nuclear test operations conducted at the Nevada Test Site. The function and role of this Advisory Groups is threefold.

First, as a multi-disciplinary group of experts, the Group is expected to provide effective and objective working-level advice and recommendations to the Manager, NV, in the planning, organization, and technical direction of the project. Secondly, the Group will review the activities of the project. Thirdly, the Group will forward copies of all reports on the progress of the project including the identification of problem areas, if any, to both the Secretary of Energy and to the Manager, NV. The Manager, NV, will maintain management and administrative supervision of the project. The group will act in an advisory and review capacity to the project. The Secretary will receive and review reports of the group and, where appropriate, resolve problems which might arise.

5. ENERGY RESEARCH ADVISORY BOARD

Objectives: To advise the Secretary, the Deputy Secretary, the Under Secretary of Energy, the Director of Energy Research and the Assistant Secretary Policy, Safety, and Environment, on overall research and development conducted in DOE and to provide long-range guidance in these areas to the Department.

6. FOSSIL ENERGY ADVISORY COMMITTEE (established by Public Law 86-599)

Objectives: (1) to provide advice and counsel in developing through research, new and more efficient methods of mining, preparing and utilizing coal; (2) to assist in the examination and evaluation of all coal research programs, proposals, and contracts and to assure the avoidance of duplicative research (Pursuant to Subsection (3) of Section 2 of Public Law 86-599, July 7, 1960 (74 Stat. 336)).

7. HEALTH AND ENVIRONMENTAL RESEARCH ADVISORY COMMITTEE

Objectives: To conduct periodic reviews of elements of the Health and Environmental Research Program and provide advice on long-range plans, priorities, and strategies to address more effectively the scientific aspects of energy-related health and environmental issues of departmental policies and programs. To provide advice on appropriate levels of funding to develop those plans, priorities, and strategies and to help maintain appropriate balance between competing elements of the program.

8. HIGH ENERGY PHYSICS ADVISORY PANEL

Objectives: To consider and provide advice and guidance on a continuing basis to the Secretary, through the Director of Energy Research, on the national high energy physics research program including: (a) periodic reviews of the program and recommendation of any changes considered desirable on the basis of scientific and technological advances or other factors; (b) advice on long-range plans, priorities and strategies for the national high energy physics program; (c) advice on recommended appropriate levels of funding to assure a world leadership position, and to help maintain appropriate balance between competing elements of the program; and (d) advice and guidance of any issues relating to the program as requested by the Secretary of the Director of Energy Research.

9. MAGNETIC FUSION ADVISORY COMMITTEE

Objectives: To provide advice and recommendations on a continuing basis to the Secretary, through the Director of Energy Research, including: (a) periodic reviews of elements of the program and recommendation of any changes considered desirable on the basis of scientific and technological advances or other factors; (b) advice on long-range plans, priorities, and strategies to demonstrate the scientific and engineering feasibility of fusion; (c) advice on recommended appropriate levels of funding to develop those strategies and to help maintain appropriate balance between competing elements of the program; (d) advice and guidance on any issues relating to the program as requested by the Secretary or the Director of Energy Research.

10. NATIONAL ENERGY EXTENSION SERVICE ADVISORY BOARD (established by Public Law 95-39)

Objectives: To carry on a continuing review of the comprehensive Energy Extension Service program and approved plans of the Governors of each state for implementing Energy Extension Service activities. The purpose of this review is to advise the Director of Energy Extension Service, the Secretary of Energy, and the Congress on the effectiveness of this program and the plans in achieving the objectives of the National Energy Extension Service Act (Public Law 95-39, Title V), and to determine how their operation might be improved in furtherance of such objectives.

11. NATIONAL PETROLEUM COUNCIL

Objectives: To provide advice, information, and recommendations to the Secretary of Energy on matters relating to oil and gas or the oil and gas industries.

12. SOLAR PHOTOVOLTAIC ENERGY ADVISORY COMMITTEE (established by Public Law 95-590, Section 9)

Objectives: To advise the Secretary on the scope of pace of research and development with respect to solar photovoltaic energy systems; the need for and timing of solar photovoltaic energy systems demonstration projects; the need for change in any research, development, or demonstration program established under this Act; and the economic, technological and environmental consequences of the use of solar photovoltaic energy systems.

13. TECHNICAL PANEL ON MAGNETIC FUSION OF THE ENERGY RESEARCH ADVISORY BOARD (established by Public Law 96-386)

Objectives: The Panel shall perform a review of the conduct of the national magnetic fusion energy program and make recommendations on the following items, among others; (a) the preparation of the 5-year program plan required by Section 5 of the Act; (b) the preparation of the 5-year program plan required by Section 5 of the Act; (b) the type of future facilities needed to meet the goals of the Act along with their projected completion dates; to meet the goals of the Act along with

their projected completion dates; (c) the adequacy of participation by universities and industry in the program; (d) the adequacy of international cooperation in magnetic fusion and any problems associated therewith; and (e) institutional, environmental, and economic factors limiting, or prospectively limiting, efforts to achieve commercial application of magnetic fusion energy systems.

ATTACHMENT B

List of Advisory Committee Memberships

ADVISORY COMMITTEE ON FEDERAL ASSISTANCE
FOR ALTERNATIVE FUELS DEMONSTRATION FACILITIES
August 1984

Honorable Allen I. Olson
Governor of North Dakota
Bismarck, North Dakota 58505

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ADVISORY PANEL ON ALTERNATIVE MEANS OF FINANCING AND MANAGING RADIOACTIVE WASTE FACILITIES

August 1984

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SOLAR PHOTOVOLTAIC ENERGY ADVISORY COMMITTEE

Inactive - no members

TECHNICAL PANEL ON MAGNETIC FUSION OF THE ENERGY RESEARCH ADVISORY BOARD

September 12, 1983

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4. **For the period FY 1981 - FY 1985, what level of funding was provided each of the advisory committee's identified in question 3 above?**

Answer: Attachment C is a copy of a consolidated portion of a DOE Annual Report listing DOE committee costs for Calendar Year 1981. Those which are still in existence are highlighted.

Attachment D are copies of portions of the DOE Annual Report listing costs for Calendar Year 1982 for each of the above committees which was in existence during that period.

Attachment E are copies of portions of the DOE Annual Report listing costs for FY 83 and cost projections for FY 84 for each of the above committees which was in existence during that period.

Attachment F are copies of 2 charters for DOE committees established since the above reports were prepared. Their proposed annual operating costs are estimated in paragraph 7 of each charter.

The DOE FY 84 Annual Report is in preparation stages. Cost figures for FY 85 have not been estimated at the present time.

[See instructions on reverse]

Interagency Report Control No. 1121-GSA-AI

ANNUAL REPORT ON FEDERAL ADVISORY COMMITTEES SUMMARY SHEET

1. DEPARTMENT OR AGENCY: Department of Energy

2. CALENDAR YEAR: 1981

3. EXACT NAME OF ADVISORY COMMITTEE (List alphabetically. See SF 248, Block 3. Indent and list subcommittees or other subgroups under parent committee.)	STATUS THIS CY			ESTABLISHMENT AUTHORITY					COMMITTEE TYPE			TOTAL NUMBER REPORTS	MEETINGS			PERSON-YEARS FED. STAFF SUP.		COSTS		TOTAL NUMBER OF MEMBERS DURING YEAR
	a. New	b. Existing at year end	c. Terminated	a. Directed by law	b. Authorized by law	c. Agency Authority	d. Presidential directive		a. Ad Hoc	b. Continuing	c. Presidential		a. TOTAL OPEN	b. TOTAL CLOSED	c. TOTAL PART. CLOSED	CURRENT YEAR (Whole Numbers and Fractions)	NEXT YEAR	TOTAL ANNUAL COST CURRENT YEAR (Whole dollars)	TOTAL ANNUAL COST NEXT YEAR (Whole dollars)	
	SF 248 Block 4			SF 248 Block 5					SF 248 Block 6			SF 248 Block 13	SF 248 Block 14			SF 248 Block 15A		SF 248 Block 15B		SF 249 Block 4A
* Advisory Committee on Atmospheric Carbon Dioxide			X			X				X		0	0	0	0	0	0	0	0	11
Consumer Affairs Advisory Committee		X				X				X		0	0	0	0	0	0	0	0	36
DOE/NSF Nuclear Science Advisory Committee 1/		X				X				X		1	3	0	0	1/4	1/4	51,174	50,000	17
Dose Assessment Advisory Group		X				X				X		0	3	0	0	2	2	116,424	130,200	17
* Energy Policy Task Force	X		X			X			X			1	2	0	0	1/4	0	3,745	0	22
Energy Research Advisory Board		X				X				X		3	4	0	0	5	5	1,131,500	1,245,000	26
Solar Photovoltaic Energy Adv. Comm. of the Energy Research Advisory Board		X		X						X		1	3	0	0	2/4	2/4	51,000	51,000	11
Environmental Advisory Comm.		X				X				X		0	4	0	0	2/4	1 3/4	45,966	143,325	25
* Federal Photovoltaic Utilization Program Adv. Comm.			X	X						X		0	0	0	0	0	0	0	0	24
* Food Industry Advisory Comm.			X			X				X		0	0	0	0	0	0	0	0	26

(If continuation of this summary listing is required, use this same form SF 250. No continuation sheet exists for this form.)

STANDARD FORM 250 (REV. 3-81)
PRESCRIBED BY GSA FPMR (41 CFR) 101-11.1

(See instructions on reverse)

Interagency Report Control No. 1121-GSA-AN

ANNUAL REPORT ON FEDERAL ADVISORY COMMITTEES SUMMARY SHEET

1. DEPARTMENT OR AGENCY: Department of Energy

2. CALENDAR YEAR: 1981

3. EXACT NAME OF ADVISORY COMMITTEE (List alphabetically. See SF 248, Block 3. Indent and list subcommittees or other subgroups under parent committee.)	STATUS THIS CY			ESTABLISHMENT AUTHORITY				COMMITTEE TYPE			TOTAL NUMBER REPORTS	MEETINGS			PERSON-YEARS FED. STAFF SUP.		COSTS		TOTAL NUMBER OF MEMBERS DURING YEAR
	a. New	b. Existing at year end	c. Terminated	a. Directed by law	b. Authorized by law	c. Agency Authority	d. Presidential directive	a. Ad Hoc	b. Continuing	c. Presidential		a. TOTAL OPEN	b. TOTAL CLOSED	c. TOTAL PART. CLOSED	CURRENT YEAR (Whole Numbers and Fractions)	NEXT YEAR (Whole Numbers and Fractions)	TOTAL ANNUAL COST CURRENT YEAR (Whole dollars)	TOTAL ANNUAL COST NEXT YEAR (Whole dollars)	
	SF 248 Block 4			SF 248 Block 6				SF 248 Block 8			SF 248 Block 13	SF 248 Block 14			SF 248 Block 15A		SF 248 Block 16B		SF 249 Block 4A
Fossil Energy Advisory Committee		X		X					X		0	0	0	0	1/4	2	10,000	125,000	22
* Fuel Oil Marketing Advisory Committee			X			X			X		0	0	0	0	0	0	0	0	36
* Gasoline Marketing Advisory Committee			X			X			X		0	0	0	0	0	0	0	0	29
High Energy Physics Advisory Panel		X				X			X		1	5	0	0	3/4	2/4	140,750	52,500	20
* Local Government Energy Policy Advisory Committee			X			X			X		0	0	0	0	0	0	0	0	30
Minority Advisory Committee on Energy	X	X				X			X		0	0	0	0	0	1	0	75,000	0
National Energy Extension Service Advisory Board		X		X					X		1	1	0	0	1/4	1/4	22,830	23,500	14
National Petroleum Council		X					X		X		5	6	0	0	3/4	2/4	82,525	102,000	122
* State Planning Council on Radioactive Waste Management			X				X	X		X	1	2	0	0	1/4	0	723,355	0	21

(If continuation of this summary listing is required, use this same form SF 250. No continuation sheet exists for this form.)

STANDARD FORM 250 (REV. 9-81)
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(See instructions on reverse)

Interagency Report Control No. 1121-GSA-A

ANNUAL REPORT ON FEDERAL ADVISORY COMMITTEES SUMMARY SHEET

1. DEPARTMENT OR AGENCY: Department of Energy

2. CALENDAR YEAR: 1981

3. EXACT NAME OF ADVISORY COMMITTEE (List alphabetically. See SF 248, Block 3. Indent and list subcommittees or other subgroups under parent committee.)	STATUS THIS CY			ESTABLISHMENT AUTHORITY				COMMITTEE TYPE			TOTAL NUMBER REPORTS	MEETINGS			PERSON-YEARS		COSTS		TOTAL NUMBER OF MEMBERS DURING YEAR
	a. New	b. Existing at year end	c. Terminated	a. Directed by law	b. Authorized by law	c. Agency Authority	d. Presidential directive	a. Ad Hoc	b. Continuing	c. Presidential		a. TOTAL OPEN	b. TOTAL CLOSED	c. TOTAL PART. CLOSED	FED. STAFF SUP. CURRENT YEAR (Whole Numbers and Fractions)	FED. STAFF SUP. NEXT YEAR (Whole Numbers and Fractions)	TOTAL ANNUAL COST CURRENT YEAR (Whole dollars)	TOTAL ANNUAL COST NEXT YEAR (Whole dollars)	
	SF 248 Block 4			SF 248 Block 5				SF 248 Block 6			SF 248 Block 13	SF 248 Block 14			SF 248 Block 15A		SF 248 Block 15B		SF 249 Block 4A
* Subtotal for Terminated Committees	1	0	8	1	0	6	1	2	6	1	2	4	0	0	2/4	0	727,100	0	199
Subtotal for Committees in Existence at End of Year	1	11	0	3	0	7	1	0	11	0	12	29	0	0	10 1/4	13 3/4	1,652,169	1,997,525	310
TOTAL	2	11	8	4	0	13	2	2	17	1	14	33	0	0	10 3/4	13 3/4	2,379,269	1,997,525	509

1/ Committee Transferred to DOE From National Science Foundation January 29, 1981

(If continuation of this summary listing is required, use this same form SF 250. No continuation sheet exists for this form.)

STANDARD FORM 250 (REV. 9-81)
PRESCRIBED BY GSA FPMR (41 CFR) 101-11.

ATTACHMENT D

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include Items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): Advisory Committee on Federal Assistance for Alternative Fuel Demonstration Facilities

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete Item 5B.): ☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate): ☐ A. AD HOC ☐ B. CONTINUING ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS: ☐ AGENCY AUTHORIZATION ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY: ☐ PRESIDENT ☐ OTHER (Specify) ☐ AGENCY HEAD

9B. LENGTH OF APPOINTMENT: ☐ INDEFINITE ☐ OTHER (Specify)

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
0	

11. NUMBER OF MEMBERS

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
NA	10			.1

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
1	0	0	1	September 28

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 0
	(2) STAFF		0	0
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	6,915.99	21,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	619.00	4,000
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			15,625.75	48,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			179.65	700
E. OTHER (Graphics, printing, SLUC, etc.)			1,133.52	3,600
F. TOTAL ▶			$ 24,473.91	$ 77,300

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR? ☐ YES ☒ NO (If "YES" is checked, complete Items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed): ☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE

NOTE: If box 16B or 16C is checked, complete Items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE? ☐ YES ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED? ☐ YES ☐ NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include Items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): Dose Assessment Advisory Group

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent): July 15, 1982

5A. ESTABLISHMENT AUTHORITY (Check only one and complete Item 5B.): [ ] SPECIFICALLY DIRECTED BY LAW [ ] AUTHORIZED BY LAW [X] AGENCY AUTHORITY [ ] PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY: DOE Determination to Establis
45 FR 46848, 7-11-80

6. COMMITTEE TYPE (Check either A or B, and C if appropriate): [ ] A. AD HOC [X] B. CONTINUING [ ] C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS: To provide advice to the Department of Energy in determining the radiation doses to individuals in Utah, Nevada, and Arizona resulting from fallout from atmospheric nuclear testing.

8A. BASIS FOR COMPENSATION OF MEMBERS: NA
[ ] AGENCY AUTHORIZATION [ ] STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY: [ ] PRESIDENT [ ] OTHER (Specify) [X] AGENCY HEAD

9B. LENGTH OF APPOINTMENT: [ ] INDEFINITE [X] OTHER (Specify) 2 years

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR:

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
1	Secretary's Executive Summary (5/82)

11. NUMBER OF MEMBERS:

A. BEGINNING (1-1-83)	B. ENDING (12-31-83)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
17	16			2

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
1	0	0	1	May 6-7

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$	$
	(2) STAFF		97,020.17	100,000
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	19,000.00	25,000
		(b) STAFF		
	(2) FEDERAL	(a) MEMBER		
		(b) STAFF		
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES				
D. RENTAL OF NON-FEDERAL MEETING FACILITIES				
E. OTHER (Graphics, printing, SLUC, etc.)			15,096.00	36,000
F. TOTAL ▶			$ 131,116.17	$ 161,000

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR? [ ] YES [X] NO (If "YES" is checked, complete Items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed): [X] A. CONTINUE [ ] B. MERGE [ ] C. TERMINATE

NOTE: If box 16B or 16C is checked, complete Items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE? [ ] YES [ ] NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED? [ ] YES [ ] NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS. Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include Items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): Energy Research Advisory Board

SECTION A — *(Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)*

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete Item 5B.)
- ☐ SPECIFICALLY DIRECTED BY LAW
- ☐ AUTHORIZED BY LAW
- ☐ AGENCY AUTHORITY
- ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate)
- ☐ A. AD HOC
- ☐ B. CONTINUING
- ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS
- ☐ AGENCY AUTHORIZATION
- ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY
- ☐ PRESIDENT
- ☐ OTHER (Specify)
- ☐ AGENCY HEAD

9B. LENGTH OF APPOINTMENT
- ☐ INDEFINITE
- ☐ OTHER (Specify)

SECTION B — *(Complete this section for ALL committees in existence during calendar year 82)*

10. REPORTS DURING CALENDAR YEAR:

A. TOTAL NUMBER OF ALL REPORTS: 4

B. REPORT TITLES AND DATES (Provide only those not previously submitted):
Interim Report on Multiprogram Laboratories (4/82)
Advanced Isotope Separation (5/82)
Final Report of Multiprogram Laboratories (9/82)
Solar Energy R&D: Federal and Private Sector Roles (9/82)

11. NUMBER OF MEMBERS

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
22	22			7¼

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
5	0	1	5	February 4-5, June 3-4, November 4-5, April 8-9, September 9-10

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 0
	(2) STAFF		280,000	295,000
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	160,000	175,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	14,000	15,000
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			600,000	650,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, SLUC, etc.)			30,000	30,000
F. TOTAL ▶			$1,084,000	$1,165,000

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR?
- ☐ YES
- ☒ NO (If "YES" is checked, complete Items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed)
- ☒ A. CONTINUE
- ☐ B. MERGE
- ☐ C. TERMINATE

NOTE: If box 16B or 16C is checked, complete Items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?
- ☐ YES
- ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED?
- ☐ YES
- ☐ NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): Fossil Energy Advisory Committee

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete item 5B.)
- [ ] SPECIFICALLY DIRECTED BY LAW
- [ ] AUTHORIZED BY LAW
- [ ] AGENCY AUTHORITY
- [ ] PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate)
- [ ] A. AD HOC
- [ ] B. CONTINUING
- [ ] C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS
- [ ] AGENCY AUTHORIZATION
- [ ] STATUTORY (If checked, complete item 8B)

8B. STATUTE:

8A. TYPE OF COMMITTEE APPOINTMENT BY
- [ ] PRESIDENT
- [ ] OTHER (Specify)
- [ ] AGENCY HEAD

9B. LENGTH OF APPOINTMENT
- [ ] INDEFINITE
- [ ] OTHER (Specify)

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR:

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
0	

11. NUMBER OF MEMBERS:

A. BEGINNING (1-1-83)	B. ENDING (12-31-83)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
22	22			0

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
0	0	0	0	

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 3,330
	(2) STAFF		0	71,670
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	0	50,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	0	3,000
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			0	7,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	5,000
E. OTHER (Graphics, printing, SLUC, etc.)			0	10,000
F. TOTAL ▶			$ 0	$150,000

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR?
- [ ] YES
- [X] NO (If "YES" is checked, complete items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed)
- [X] A. CONTINUE
- [ ] B. MERGE
- [ ] C. TERMINATE

NOTE: If box 16B or 16C is checked, complete items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?
- [ ] YES
- [ ] NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED?
- [ ] YES
- [ ] NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO. 0204-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): High Energy Physics Advisory Panel

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete Item 5B.): ☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate): ☐ A. AD HOC ☐ B. CONTINUING ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS: ☐ AGENCY AUTHORIZATION ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY: ☐ PRESIDENT ☐ AGENCY HEAD ☐ OTHER (Specify)

9B. LENGTH OF APPOINTMENT: ☐ INDEFINITE ☐ OTHER (Specify)

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
1	Report of the Subpanel on Long Range Planning for the U.S. High Energy Physics Program of the High Energy Physics Advisory Panel (1/82)

11. NUMBER OF MEMBERS

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
15	14			.5

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
5	0	0	5	January 14-16, May 10-11, November 11-12, February 19-20, August 9-10

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 0
	(2) STAFF		19,000	30,000
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	29,835	50,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	2,815	20,000
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			5,400	0
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, SF,UC, etc.)			800	500
TOTAL			$ 57,850	$ 100,500*

*$100K estimate for FY83 above $50K quoted in Charter due to anticipated Long Range Subpanel to be working during this perio

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR? ☐ YES ☒ NO (If "YES" is checked, complete Items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed.) ☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE

NOTE: If box 16B or 16C is checked, complete Items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE? ☐ YES ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED? ☐ YES ☐ NO

GENERAL SERVICES ADMINISTRATION

GSA FORM T820-A PAGE 1 (12-82)

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REPORT: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): Magnetic Fusion Advisory Committee

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent)

5A. ESTABLISHMENT AUTHORITY (Check only one and complete item 5B.)
- ☐ SPECIFICALLY DIRECTED BY LAW
- ☐ AUTHORIZED BY LAW
- ☐ AGENCY AUTHORITY
- ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY

6. COMMITTEE TYPE (Check either A or B, and C if appropriate)
- ☐ A. AD HOC ☐ B. CONTINUING
- ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS

8A. BASIS FOR COMPENSATION OF MEMBERS
- ☐ AGENCY AUTHORIZATION
- ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE

9A. TYPE OF COMMITTEE APPOINTMENT BY
- ☐ PRESIDENT ☐ OTHER (Specify)
- ☐ AGENCY HEAD

9B. LENGTH OF APPOINTMENT
- ☐ INDEFINITE
- ☐ OTHER (Specify)

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
1	Report on Evaluation of Magnetic Confinement Concepts (11/82)

11. NUMBER OF MEMBERS

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
NA	16			½

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
3	0	0	3	June 1-2, November 1, August 30-31

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 0
	(2) STAFF		16,000	21,000
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	160,000	160,000
		(b) STAFF		
	(2) FEDERAL	(a) MEMBER		
		(b) STAFF	2,000	4,000
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES				
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, SLUC, etc.)			2,000	4,000
F. TOTAL ▶			$180,000	$189,000

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR?
- ☐ YES ☒ NO (If "YES" is checked, complete Items 15B and 15C)

15B. TERMINATION AUTHORITY

15C. TERMINATION DATE

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed)
- ☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE

NOTE: If box 15B or 15C is checked, complete Items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE? ☐ YES ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED? ☐ YES ☐ NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include Items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): National Energy Extension Service Advisory Board

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete Item 5B.): ☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate): ☐ A. AD HOC ☐ B. CONTINUING ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS: ☐ AGENCY AUTHORIZATION ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY: ☐ PRESIDENT ☐ AGENCY HEAD ☐ OTHER (Specify)

9B. LENGTH OF APPOINTMENT: ☐ INDEFINITE ☐ OTHER (Specify)

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR:

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
1	Third Annual Report to Congress and the Secretary of Energy on the Nationwide Energy Extension Service Program (1/82)

11. NUMBER OF MEMBERS:

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
14	16			.4

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
1	0	0	1	December 6-7

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 0
	(2) STAFF		15,000.00	15,000.00
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	10,000.00	20,000.00
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	0	0
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			6,500.00	9,200.00
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			2,000.00	3,500.00
E. OTHER (Graphics, printing, BLUC, etc.)			0	0
		F. TOTAL ▶	$ 33,500.00	$ 47,700.00

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR? ☐ YES ☒ NO (If "YES" is checked, complete Items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed)

NOTE: If box 16B or 16C is checked, complete Items 17A, 17B and 18.

☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE? ☐ YES ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED? ☐ YES ☐ NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS. Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach separate sheets and key answers to item numbers and include Items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REVIEW: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): National Petroleum Council

SECTION A – (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete Item 5B.)
- ☐ SPECIFICALLY DIRECTED BY LAW
- ☐ AUTHORIZED BY LAW
- ☐ AGENCY AUTHORITY
- ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate)
- ☐ A. AD HOC
- ☐ B. CONTINUING
- ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS
- ☐ AGENCY AUTHORIZATION
- ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY
- ☐ PRESIDENT
- ☐ OTHER (Specify)
- ☐ AGENCY HEAD

9B. LENGTH OF APPOINTMENT
- ☐ INDEFINITE
- ☐ OTHER (Specify)

SECTION B – (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
3	Environmental Conservation (4/82) Enhanced Oil Recovery (Progress Report) (12/82) Third World Petroleum Development (12/82)

11. NUMBER OF MEMBERS

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
113	114			1

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)		
6	0	0	6	March 9	August 11	October 29
				April 21	October 19	December 1

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
			$	$
A. COMPENSATION	(1) NON-FEDERAL MEMBER			
	(2) STAFF		25,000	22,000
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	0	0
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	8,000	20,000
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			0	0
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, SLUC, etc.)			1,000	1,000
F. TOTAL ▶			$ 34,000	$ 43,000

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR?
- ☐ YES
- ☒ NO (If "YES" is checked, complete Item 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box only if not previously submitted, or if recommendation has changed)
- ☒ A. CONTINUE
- ☐ B. MERGE
- ☐ C. TERMINATE

NOTE: If box 16B or 16C is checked, complete Items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE? ☐ YES ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED? ☐ YES ☐ NO

REVIEW OF FEDERAL ADVISORY COMMITTEES

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during calendar year 82 (1-1-82 to 12-31-82). If additional space is necessary, attach seperate sheets and key answers to item numbers and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. DATE OF THIS REPORT: December 30, 1982

3. NAME OF COMMITTEE (Include subcommittee, if appropriate): Solar Photovoltaic Energy Advisory Committee

SECTION A — (Complete this section ONLY if committee has been established or reestablished since 6-30-82, or if any information previously submitted has changed.)

4. DATE ESTABLISHED OR LAST REESTABLISHED OR RENEWED (Most recent):

5A. ESTABLISHMENT AUTHORITY (Check only one and complete item 5B.)
- ☐ SPECIFICALLY DIRECTED BY LAW
- ☐ AUTHORIZED BY LAW
- ☐ AGENCY AUTHORITY
- ☐ PRESIDENTIAL AUTHORITY

5B. SPECIFIC ESTABLISHMENT AUTHORITY:

6. COMMITTEE TYPE (Check either A or B, and C if appropriate)
- ☐ A. AD HOC
- ☐ B. CONTINUING
- ☐ C. PRESIDENTIAL

7. BRIEF STATEMENT OF FUNCTIONS:

8A. BASIS FOR COMPENSATION OF MEMBERS
- ☐ AGENCY AUTHORIZATION
- ☐ STATUTORY (If checked, complete Item 8B)

8B. STATUTE:

9A. TYPE OF COMMITTEE APPOINTMENT BY
- ☐ PRESIDENT
- ☐ OTHER (Specify)
- ☒ AGENCY HEAD

9B. LENGTH OF APPOINTMENT
- ☐ INDEFINITE
- ☐ OTHER (Specify)

SECTION B — (Complete this section for ALL committees in existence during calendar year 82)

10. REPORTS DURING CALENDAR YEAR:

A. TOTAL NUMBER OF ALL REPORTS	B. REPORT TITLES AND DATES (Provide only those not previously submitted)
0	

11. NUMBER OF MEMBERS:

A. BEGINNING (1-1-82)	B. ENDING (12-31-82)	C. AUTHORIZED (Complete only if not previously submitted)	D. COMPENSATED (Complete only if not previously submitted)	12. STAFF SUPPORT YEARS DURING CALENDAR YEAR
13	13			1.6

13. MEETINGS DURING CALENDAR YEAR

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL	E. DATES OF MEETINGS (Month, Day)
0	0	0	0	

14. COMMITTEE COST

DESCRIPTION			ACTUAL FOR CALENDAR YEAR 82 (1-1-82 to 12-31-82)	ESTIMATE FOR FISCAL YEAR 83 (10-1-82 to 9-30-83)
A. COMPENSATION	(1) NON-FEDERAL MEMBER		$ 0	$ 0
	(2) STAFF		5,000	2,500
B. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBER	0	0
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBER	0	0
		(b) STAFF	0	0
C. FEES FOR CONSULTANTS, EXPERTS AND OTHER NON-FEDERAL PERSONNEL SERVICES			0	0
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, SLUC, etc.)			0	0
F. TOTAL ▶			$ 5,000	$ 2,500

15A. HAS THIS COMMITTEE BEEN TERMINATED DURING CALENDAR YEAR?
- ☐ YES ☒ NO (If "YES" is checked, complete items 15B and 15C)

15B. TERMINATION AUTHORITY:

15C. TERMINATION DATE:

16. AGENCY RECOMMENDATION FOR COMMITTEE (Check appropriate box)
- ☒ A. CONTINUE
- ☐ B. MERGE
- ☐ C. TERMINATE

NOTE: If box 16B or 16C is checked, complete items 17A, 17B and 18.

17A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?
- ☐ YES ☐ NO

17B. IS SUCH LEGISLATION PENDING OR ENACTED?
- ☐ YES ☐ NO

ATTACHMENT E

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: Advisory Committee on Federal Assistance for Alternative Fuels Demonstration Facilities

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	1/27/82	1/27/84	—

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete Items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
☐ YES ☒ NO	—	—

NOTE: If box 8B or 8C is checked, complete Items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☒ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
P.L. 93-577 as amended by P.L. 95-238 42 USC 5919	2/25/78	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☒ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☐ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete Item 16B)	NA	$ NA

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)

18. LENGTH OF APPOINTMENT
☐ INDEFINITE ☒ SPECIFIC TERM 24 MO. (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
0	10	11	11	—	—

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
2			2	2/25/83 6/28/83

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ -0-	$ -0-
	(2) FEDERAL MEMBERS (Prorated salary)		-0-	-0-
	(3) FEDERAL STAFF (Prorated salary)		4500.00	6,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			27173.00	43,000
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	7716.13	13,000
		(b) STAFF	-0-	-0-
	(2) FEDERAL	(a) MEMBERS	-0-	-0-
		(b) STAFF	1067.94	2,500
D. [illegible] FEDERAL MEETING FACILITIES			-0-	-0-
E. OTHER (Graphics, printing, photocopying, mailing, BLUC, etc.)			1993.00	2,700
		F. TOTAL ▶	$ 42450.07	$ 67,200
23. FEDERAL STAFF SUPPORT YEARS (Express in person years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			.12	.15

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: Advisory Panel on Alternative Means of Financing and Managing Radioactive Waste Facilities

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
[X] YES [ ] NO	6-24-83	NA	See item 26. 3-7-84

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
[ ] YES [X] NO		

NOTE: If box 8B or 8C is checked, complete items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
[X] A. CONTINUE [ ] B. MERGE [ ] C. TERMINATE	[ ] YES [ ] NO	[ ] YES [ ] NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
[ ] SPECIFICALLY DIRECTED BY LAW [ ] AUTHORIZED BY LAW [X] AGENCY AUTHORITY [ ] PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
DOE Determination to Establish 48 FR 26520	6-8-83	[X] A. AD HOC [ ] B. CONTINUING [ ] C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
[X] MAJOR NATIONAL POLICY/ISSUE ADVISORY [ ] PROGRAM ADVISORY [ ] SCIENTIFIC/TECHNICAL [ ] GRANT REVIEW [ ] OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
[ ] AGENCY AUTHORIZATION [ ] STATUTORY (If statutory, complete item 16B)		$

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)	18. LENGTH OF APPOINTMENT
[ ] PRESIDENTIAL [X] AGENCY HEAD [ ] CONGRESSIONAL [ ] OTHER (Specify)	[ ] INDEFINITE [X] SPECIFIC TERM 9 (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
0	0	0	0	Approx. 10	

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
0	0	0	0	

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 0
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		6,000	40,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			0	0
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	0	45,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	0	2,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			0	15,000
		F. TOTAL ▶	$ 6,000	$ 102,000
23. FEDERAL STAFF SUPPORT YEARS (Express in person years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in item 22A(3), above.) ▶			.10	.65

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: DEPARTMENT OF ENERGY

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: DOSE ASSESSMENT ADVISORY GROUP (DAAG)

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	July 15, 1982	N/A	July 15, 1984

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete Items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
☐ YES ☒ NO		

NOTE: If box 8B or 8C is checked, complete Items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☒ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
DOE determination to establish 45 FR 46848. 7/11/80	7/11/80	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☐ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☒ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete Item 16B)		$ -0-

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)	18. LENGTH OF APPOINTMENT
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)	☐ INDEFINITE ☒ SPECIFIC TERM (Indicate no. of months) 24

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
2	16	16	16	20	-0-

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
2			2	January 6 and 7 May 19 and 20

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$	$
	(2) FEDERAL MEMBERS (Prorated salary)			
	(3) FEDERAL STAFF (Prorated salary)		74,701.50	74,701.50
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)				
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	26,029.00	52,058.00
		(b) STAFF		
	(2) FEDERAL	(a) MEMBERS		
		(b) STAFF		
D. RENTAL OF NON-FEDERAL MEETING FACILITIES				
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			14,000.00	20,700.00
		F. TOTAL ▶	$114,630.50	$157,459.50
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			1.85	1.85

GENERAL SERVICES ADMINISTRATION — GSA FORM T-220-B (9-83)

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: Energy Research Advisory Board

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	6/19/82	6/19/84	N/A

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
☐ YES ☒ NO		

NOTE: If box 8B or 8C is checked, complete items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☒ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
DOE Notice of Establishment 43 FR 24130	6/2/78	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☐ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☐ PROGRAM ADVISORY ☒ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete item 16B)	Members are not compensated	

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)

18. LENGTH OF APPOINTMENT: ☐ INDEFINITE ☒ SPECIFIC TERM (Indicate no. of months) 12 Months

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
4	25	23	25	approx. 25	None

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
4			4	Nov. 4-5, 1982; May 5-6, 1983; Feb. 3-4, 1983; Aug 3,4-5, 1983

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ -0-	$ -0-
	(2) FEDERAL MEMBERS (Prorated salary)		-0-	-0-
	(3) FEDERAL STAFF (Prorated salary)		150,000	150,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			-0-	-0-
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	40,000	40,000
		(b) STAFF	-0-	-0-
	(2) FEDERAL	(a) MEMBERS	-0-	-0-
		(b) STAFF	7,000	7,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			-0-	-0-
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			15,000	15,000
		F. TOTAL ▶	$212,000	$212,000
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in item 22A(3), above.)		▶	5.	5.

GSA [illegible]

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy
2. FISCAL YEAR: 1983
3. NAME OF COMMITTEE: Fossil Energy Advisory Committee

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	8-3-83	8-3-85	

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete Items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
☐ YES ☒ NO		

NOTE: If box 8B or 8C is checked, complete Items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☒ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
Section 2, P.L. 86-599 (74 Stat. 336) 30 U.S.C. Section 662 and 663	7-6-70	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☐ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☒ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☒ STATUTORY (If statutory, complete Item 16B)	30 U.S.C. Section 663	$ 50.00

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)

18. LENGTH OF APPOINTMENT
☐ INDEFINITE ☒ SPECIFIC TERM 24 (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
0	0	0	0	24	0

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
0	0	0	0	

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 1,665
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		0	35,835
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			0	3,500
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	0	25,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	0	1,500
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	2,500
E. OTHER (Graphics, printing, photocopying, mailing, BLUC, etc.)			0	5,000
		F. TOTAL ▶	$ 0	$ 75,000
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (e.g., 0.90). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			.0	.5

GSA FORM T-320B (8-83)

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 8304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U.S. Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: High Energy Physics Advisory Panel

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	Jan. 27, 1983	Jan. 27, 1985	
8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete Items 8B and 8C)	**8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)**		**8C. ACTUAL TERMINATION DATE**
☐ YES ☒ NO	n/a		n/a

NOTE: If box 8B or 8C is checked, complete Items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☒ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
Atomic Energy Commission Action	Jan. 13, 1967	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☐ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☒ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete Item 16B) n/a	n/a	$ n/a

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)	18. LENGTH OF APPOINTMENT
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)	☐ INDEFINITE ☒ SPECIFIC TERM 12 mo. (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
1	15	15	15	~ 15	0

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
3	0	0	3	11/11-12/82, 2/7-8/83, 7/11-12/83

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 0
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		19,500	23,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			3,600	5,500
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	13,000	16,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	2,000	3,500
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Telephone, printing, photocopying, mailing, SLUC, etc.)			500	600
		F. TOTAL ▶	$ 38,600	$ 48,600
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth e.g., 0.00). Figure should correspond to dollar cost in Item 22A (3), above.)		▶	.50	.50

GSA FORM T-820-B (8-83)

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: Magnetic Fusion Advisory Committee

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	5-25-82	5-25-84	

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete Items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
☐ YES ☒ NO		

NOTE: If box 8B or 8C is checked, complete Items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☒ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
42 USC Sec 9301-9312 94 Stat 1539 DOE Notice of Establishment 47 FR 23198	5-27-82	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☐ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☐ PROGRAM ADVISORY ☒ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete Item 16B)		$

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)

18. LENGTH OF APPOINTMENT
☐ INDEFINITE ☒ SPECIFIC TERM 12 (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".): 6

20. NUMBER OF MEMBERS

A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
15	16	16	16	0

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
5	0	0	5	11-1-82 5-3 & 5-4-83 9-27 & 9-28-83 1-10 & 1-11-83 8-2 & 8-3-83

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 0
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		20,000	22,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			0	0
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	30,000	32,000
		(b) STAFF	1,500	2,000
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	3,000	2,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			0	0
		F. TOTAL ▶	$ 54,500	$ 58,000
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in Item 22A (3), above.)		▶	.5	.5

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: National Energy Extension Service Advisory Board

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	6-14-82	6-14-84	
8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete items 8B and 8C)	**8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)**		**8C. ACTUAL TERMINATION DATE**
☐ YES ☒ NO			

NOTE: If box 8B or 8C is checked, complete items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one.)
☒ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
National Energy Extension Service Act, Sec. 509, P.L. 93-39 (Title 42 U.S.C. 7008)	6-3-77	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☒ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☐ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete Item 16B)		$

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)	18. LENGTH OF APPOINTMENT
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)	☐ INDEFINITE ☒ SPECIFIC TERM 12 (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
1	16	16	16	Up to 20	0

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
3	0	0	3	12-6 and 12-7-82 3-11 and 3-12-83 1-25-83

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave b'ank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 0
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		30,000	30,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			11,000	11,500
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	10,000	10,000
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	0	0
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			1,000	1,000
		F. TOTAL ▶	$ 52,000	$ 52,500
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			.4	.4

GSA FORM T-220-R (6-83)

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO.: 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: U. S. Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: National Petroleum Council

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	12/31/81	12/31/83	N/A
8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete items 8B and 8C)	**8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)**		**8C. ACTUAL TERMINATION DATE**
☐ YES ☒ NO			

NOTE: If box 8B or 8C is checked, complete items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☒ A. CONTINUE ☐ B. MERGE ☐ C. TERMINATE	☐ YES ☐ NO	☐ YES ☐ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☐ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☒ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
Letter of May 3, 1946, from President Harry S. Truman to Secretary of Interior	5-3-46	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☒ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☐ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete item 16B)		$

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)
☐ PRESIDENTIAL ☒ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)

18. LENGTH OF APPOINTMENT
☐ INDEFINITE ☒ SPECIFIC TERM 24 (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
4	115	120	131	125	0

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)		
6	0	0	6	October 19	December 1	May 18
				October 29	March 18	May 19

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 0
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		25,000	25,000
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			0	0
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	13,000	13,000
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			1,000	1,000
		F. TOTAL ▶	$39,000	$39,000
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (e.g., 0.00). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			0.50	0.50

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: Solar Photovoltaic Energy Advisory Committee

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
☐ YES ☒ NO	2-15-82	NA	1986

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
☐ YES ☒ NO		

NOTE: If box 8B or 8C is checked, complete items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
☐ A. CONTINUE ☐ B. MERGE ☒ C. TERMINATE	☒ YES ☐ NO	☐ YES ☒ NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
☒ SPECIFICALLY DIRECTED BY LAW ☐ AUTHORIZED BY LAW ☐ AGENCY AUTHORITY ☐ PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
P.L. 95-590	11-4-78	☐ A. AD HOC ☒ B. CONTINUING ☐ C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
☐ MAJOR NATIONAL POLICY/ISSUE ADVISORY ☒ PROGRAM ADVISORY ☐ SCIENTIFIC/TECHNICAL ☐ GRANT REVIEW ☐ OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
☐ AGENCY AUTHORIZATION ☐ STATUTORY (If statutory, complete item 16B)		$

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)	18. LENGTH OF APPOINTMENT
☒ PRESIDENTIAL ☐ AGENCY HEAD ☐ CONGRESSIONAL ☐ OTHER (Specify)	☐ INDEFINITE ☒ SPECIFIC TERM (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
0	0	0	0	13	0

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS:				F. DATES OF ALL MEETINGS (Month, day)
A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	
0	0	0	0	

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ 0	$ 0
	(2) FEDERAL MEMBERS (Prorated salary)		0	0
	(3) FEDERAL STAFF (Prorated salary)		0	0
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			0	0
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	0	0
	(2) FEDERAL	(a) MEMBERS	0	0
		(b) STAFF	0	0
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			0	0
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			0	0
		F. TOTAL ▶	$ 0	$ 0
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (i.e., 0.00). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			.0	.0

REVIEW OF FEDERAL ADVISORY COMMITTEE

REPORTS CONTROL NO. 0304-GSA-OT

INSTRUCTIONS: Complete one form for EACH committee in existence at any time during fiscal year (10-1 to 9-30). Cite ALL dates in numerals (Month, day, year). If additional space is necessary, use Section F, "Remarks" on the reverse and key answers to item numbers or attach separate sheets and include items 1, 2 and 3 on each sheet.

1. DEPARTMENT OR AGENCY: Department of Energy

2. FISCAL YEAR: 1983

3. NAME OF COMMITTEE: Technical Panel on Magnetic Fusion of the Energy Research Advisory Board

SECTION A – COMMITTEE STATUS (Complete this section for ALL committees)

4. IS THIS COMMITTEE NEW DURING FISCAL YEAR?	5. CURRENT CHARTER DATE	6. EXPECTED RENEWAL DATE	7. EXPECTED TERMINATION DATE
[X] YES [ ] NO	6/29/83	N/A	N/A

8A. HAS THIS COMMITTEE BEEN TERMINATED DURING FISCAL YEAR? (If "YES," complete items 8B and 8C)	8B. SPECIFIC TERMINATION AUTHORITY (If by law, cite U.S.C.)	8C. ACTUAL TERMINATION DATE
[ ] YES [X] NO		

NOTE: If box 8B or 8C is checked, complete items 10A and 10B and provide a brief explanation in "Remarks".

9. AGENCY RECOMMENDATION FOR COMMITTEE FOR NEXT FISCAL YEAR	10A. IS LEGISLATION REQUIRED TO MERGE OR TERMINATE?	10B. IS SUCH LEGISLATION PENDING OR ENACTED?
[X] A. CONTINUE [ ] B. MERGE [ ] C. TERMINATE	[ ] YES [ ] NO	[ ] YES [ ] NO

SECTION B – COMMITTEE AUTHORITY AND TYPE (Complete this section for ALL new committees and give brief statement of functions in "Remarks". If any information previously submitted on a continuing committee has changed, update and/or correct all items that apply.)

11. ESTABLISHMENT AUTHORITY (Check ONLY one)
[X] SPECIFICALLY DIRECTED BY LAW [ ] AUTHORIZED BY LAW [ ] AGENCY AUTHORITY [ ] PRESIDENTIAL DIRECTIVE

12. SPECIFIC ESTABLISHMENT AUTHORITY (If by law, cite U.S.C.)	13. EFFECTIVE DATE OF AUTHORITY	14. COMMITTEE TYPE (Check EITHER A or B, and C, if appropriate)
42 USC 9306 Sec. 7 of P.L. 96-386	10/7/80	[ ] A. AD HOC [X] B. CONTINUING [ ] C. PRESIDENTIAL

15. DESCRIPTION OF COMMITTEE
[ ] MAJOR NATIONAL POLICY/ISSUE ADVISORY [ ] PROGRAM ADVISORY [X] SCIENTIFIC/TECHNICAL [ ] GRANT REVIEW [ ] OTHER (Specify)

16A. BASIS FOR COMPENSATION OF MEMBERS	16B. STATUTE (U.S.C.)	16C. RATE PER MEMBER (Per day)
[ ] AGENCY AUTHORIZATION [ ] STATUTORY (If statutory, complete item 16B)		

17. TYPE OF COMMITTEE APPOINTMENT (Check ALL that apply)	18. LENGTH OF APPOINTMENT
[ ] PRESIDENTIAL [X] AGENCY HEAD [ ] CONGRESSIONAL [ ] OTHER (Specify)	[ ] INDEFINITE [ ] SPECIFIC TERM (Indicate no. of months)

SECTION C – COMMITTEE ACTIVITY DURING FISCAL YEAR (Complete this section for ALL committees)

19. TOTAL NUMBER OF REPORTS (Note: List report titles and dates in "Remarks".)	20. NUMBER OF MEMBERS				
	A. BEGINNING (10-1)	B. ENDING (9-30)	C. TOTAL SERVING (10-1 to 9-30)	D. AUTHORIZED	E. COMPENSATED
0	11	11	11	12	None

21. MEETINGS

NOTE: Meeting exemptions – For closed or partially closed meetings, list all Government in the Sunshine Act (5 U.S.C. 552b) exemptions, and number of times used in "Remarks".

NUMBER OF MEETINGS: A. OPEN	B. CLOSED	C. PARTIALLY CLOSED	D. TOTAL (A+B+C)	E. DATES OF ALL MEETINGS (Month, day)
	0	0		Aug. 30-31, 1983

SECTION D – COMMITTEE COST (Complete this section for ALL committees)

NOTE: Express costs in whole dollars. DO NOT use decimals, K, M, N/A, or leave blank. Indicate "0", if applicable)

22. DESCRIPTION			CURRENT FISCAL YEAR (Actual)	NEXT FISCAL YEAR (Estimate)
A. COMPENSATION	(1) NON-FEDERAL MEMBERS		$ -0-	$ -0-
	(2) FEDERAL MEMBERS (Prorated salary)		-0-	
	(3) FEDERAL STAFF (Prorated salary)		20,000	
B. FEES FOR SERVICES AND STAFF (Consultants, experts and other non-federal personnel)			-0-	
C. TRAVEL AND PER DIEM	(1) NON-FEDERAL	(a) MEMBERS	5,000	
		(b) STAFF	-0-	
	(2) FEDERAL	(a) MEMBERS	-0-	
		(b) STAFF	1,000	
D. RENTAL OF NON-FEDERAL MEETING FACILITIES			-0-	
E. OTHER (Graphics, printing, photocopying, mailing, SLUC, etc.)			1,000	
		F. TOTAL ▶	$ 27,000	$ -0-
23. FEDERAL STAFF SUPPORT YEARS (Express in person-years using decimals to the nearest hundredth (i.e., 0.00). Figure should correspond to dollar cost in Item 22A(3), above.) ▶			.5	.0

GSA FORM T-220.R (8-83)

ATTACHMENT F

DEPARTMENT OF ENERGY

CHARTER

AMERICAN STATISTICAL ASSOCIATION COMMITTEE ON ENERGY STATISTICS

1. Committee's Official Designation:

   American Statistical Association Committee on Energy Statistics

2. Committee's Objectives and Scope of Activities and Duties:

   The activities of the American Statistical Association Committee on Energy Statistics in support of the Energy Information Administration (EIA) include:

   a. Periodic reviews of elements of EIA information collection and analysis programs and the provision of recommendations;

   b. Advice on priorities of technical and methodological issues in the planning, operation, and review of EIA statistical programs; and

   c. Advice on matters concerning improved energy modeling and forecasting tools, particularly regarding their functioning, relevancy and results.

3. Time Period Necessary for the Committee to Carry Out Its Purpose:

   The Committee is a permanent committee of the American Statistical Association. In view of the goals and purposes for which the committee's advice is sought, its utilization is expected to be continuing in nature.

4. Official to Whom This Committee Reports:

   The Committee will report to the Administrator of the Energy Information Administration relative to the issues for which committee advice is sought.

5. Agency Responsible for Providing Necessary Support for This Committee:

   The Department of Energy. Within the DOE, primary support shall be furnished by the Energy Information Administration.

6. Description of Duties for Which the Committee is Responsible:

   The duties of the Committee as they relate to the EIA are solely advisory and are stated in Paragraph 2, above.

7. Estimated Annual Operating Costs in Dollars and Person-Years:

   $40,000; 1 person-year.

40-574 O - 85 - 55

8. Estimated Number and Frequency of Meetings:

The Committee will meet with the EIA approximately 2 times a year at six month intervals. The Committee may meet independently at times and frequencies as the Committee wishes.

9. Committee's Termination Date (If Less Than Two Years from Date of Establishment or Renewal):

Not applicable.

10. Subcommittee(s):

The American Statistical Association Committee on Energy Statistics may form subcommittees from time to time to facilitate its functioning. Ad hoc members from outside the ASA Committee on Energy Statistics may be appointed by the subcommittee chairperson to ensure the expertise necessary to conduct the subcommittee's business.

11. Members:

a. Committee members are appointed by the President of the American Statistical Association.

b. Approximate number of Committee members: 15

c. Membership terms are for a period of 3 years. Committee members may be reappointed to additional terms following review.

12. Chairperson:

The Chairperson and Vice-chairperson are elected by the Committee for a two-year term.

This Charter for utilization of the Advisory Committee named above is hereby approved on:

October 17, 1984
Date

K. Dean Kelms
Advisory Committee Management Officer

October 17, 1984
Date Filed

DEPARTMENT OF ENERGY

CHARTER

HEALTH AND ENVIRONMENTAL RESEARCH ADVISORY COMMITTEE

1. Committee's Official Designation:

   Health and Environmental Research Advisory Committee (HERAC)

2. Committee's Objectives and Scope of Activities and Duties:

   The activities of the Health and Environmental Research Advisory Committee include:

   a. Periodic reviews of elements of the Health and Environmental Research (HER) program and recommendations based thereon;

   b. Advice on long-range plans, priorities, and strategies to address more effectively the scientific aspects of energy-related health and environmental issues of departmental policies and programs;

   c. Advice on appropriate levels of funding to develop those plans, priorities and strategies and to help maintain appropriate balance between competing elements of the HER program;

   d. Advice on scientific aspects of health and environmental issues of concern to DOE as requested by the Secretary or the Director of Energy Research.

3. Time Period Necessary for the Committee to Carry Out Its Purpose:

   In view of the goals and purposes of the Committee, it is expected to be continuing in nature.

4. Official to Whom This Committee Reports:

   The Committee will report to the Secretary of Energy through the Director of Energy Research.

5. Agency Responsible for Providing Necessary Support for This Committee:

   The Department of Energy. Within the Department, primary support shall be furnished by the Office of Energy Research.

6. Description of Duties for Which the Committee is Responsible:

   The duties of the Committee are solely advisory and are stated in Paragraph 2, above.

7. Estimated Annual Operating Costs in Dollars and Person-Years:

   $75,000; 1/2 person-year.

8. Estimated Number and Frequency of Meetings:

The Committee will meet approximately 4 times a year, at least once each quarter.

9. Committee's Termination Date (If Less Than Two Years from Date of Establishment or Renewal):

Not applicable.

10. Subcommittee(s):

To facilitate the functioning of HERAC, subcommittees may be formed. The objectives of the subcommittees are to make recommendations to the parent committee with respect to particular matters related to the responsibilities of the parent committee. Ad hoc members from outside HERAC may be appointed by the subcommittee chairperson to ensure the expertise necessary to conduct the subcommittee's business.

11. Members:

a. Committee members shall be appointed by the Secretary of Energy.

b. Approximate number of Committee members: 18

c. Membership terms shall be for a period of 1 year. Committee members may be reappointed to additional terms following review.

12. Chairperson:

The Chairperson shall be appointed by the Secretary of Energy.

This Charter for the Advisory Committee named above is hereby approved on:

November 22, 1983
Date

K. Dean Helms
Advisory Committee Management Officer

November 22, 1983
Date Filed

5. **What is the function, scope and purpose of the Interagency Working Group in Strategic Minerals Policy? What agencies participate, and what is DOE's role?**

Answer: The Interagency Working Group in Strategic Minerals Policy was one of several ad hoc groups established as a result of the formation of the Cabinet Council on Natural Resources and the Environment on February 26, 1981. This task force was under the direction of the Department of Interior's (DOI) Deputy Assistant Secretary for Energy and Minerals, William P. Pendley. The efforts of this ad hoc group and others resulted in the eventual issuance of the National Materials and Minerals Program Plan and Report to Congress in April 1982. There were a number of agencies involved in the activities of the group. These included DOI, National Aeronautics and Space Administration, National Science Foundation, DOE and Department of Defense; although a number of others participated from time to time. DOE's role was limited and related primarily to providing information and data concerning DOE's R&D programs in materials.

Currently, Governmental materials research is coordinated by the Committee on Materials (COMAT) of the Federal Coordinating Council for Science, Engineering and Technology. This Committee reports to the President's Science Advisor. Dr. Alvin W. Trivelpiece, Director, Office of Energy Research, DOE, is a member of COMAT.

6. **What is the function, scope and purpose of the Intergency Program Board on Civil Operational Land Remote Sensing from Space? What agencies participate, and what is DOE's role?**

Answer: In 1983, the Secretary of Commerce replaced the Program Board on Civil Operational Land Remote Sensing from Space with the Interagency Board on Civil Operational Earth-Observing Satellite Systems. The primary purpose of the new Interagency Board is to provide policy oversight for the process of placing land remote sensing satellites in the private sector. Members of the Interagency Board include representatives from the National Security Council, Department of Defense, Department of State, Department of Justice, Department of Interior, Central Intelligence Agency, National Aeronautics and Space Administration, Office of Management and Budget, Office of Science and Technology Policy, Agency for International Development and the National Oceanic and Atmospheric Administration (Chair).

DOE participated in the defunct Program Board but does not participate on the Interagency Board.

The DOE Office of Program Analysis continues to monitor the progress of the commercialization process to ensure that land remote sensing data will continue to be available as needed for Agency missions.

7. **What activities are being carried out by the program with respect to acid rain?**

Answer: Acid precipitation phenomena and effects are among the most critical of scientific issues today, and they bear significant implications for energy research. The Director, Office of Energy Research, must be prepared to advise the Secretary on the current state-of-knowledge, the outstanding

scientific issues, and the necessary research programs to resolve these issues.

The Director, Office of Program Analysis (OPA), serves as the DOE representative to the Interagency Task Force on Acid Precipitation. He coordinates and submits the Department's research budget contribution to the interagency effort. He also provides advice in research planning and peer review of research findings. OPA staff serves on various Working Groups of the Task Force.

OPA supports the Task Force assessment activity to ensure proper scheduling of key deliverables, integration of complementary research findings, adherence to goal orientation, application of assessment methodology, and development of major scientific assessments. A Memorandum of Understanding between DOE and EPA established a special group dedicated to this purpose. One staff member is on detail to the assessment group, and funds have been made available to the National Laboratory Consortium to provide support.

OPA provides the Director, Office of Energy Research, with review, commentary and assessment of significant scientific work in acid precipitation.

When appropriate, the Office sponsors research planning or research assessment workshops.

III. UNIVERSITY RESEARCH SUPPORT (URS)

1. For the period FY 1981 - FY 1985, please provide the funding profile of the University Research Support Program.

Answer:

($ in Thousands)

University Research Support	FY 1981 BA	FY 1982 BA	FY 1983 BA	FY 1984 BA	FY 1985 BA
University/National Laboratory Cooperative Research					
University Institutional Research..	$ 2,900	$2,228	$ 0	$ 0	$ 0
University Reactor Fuel Assistance.	1,400	1,581	1,704	1,500	1,900
University Laboratory Cooperative Research.....	3,500	3,619	4,284	3,500	6,550
Energy Graduate Traineeship.....	0	1,000	0	0	0
Enery Manpower Development					
Energy Manpower Assessment.....	0	499	0	270	450
Energy Education and Training a/...	4,000	1,568	0	200	300
	$11,800	$10,495	$ 5,988	$ 5,470	$ 9,200

a/ Budgeted under Consumer Affairs, Departmental Administration Appropriation in FY 1981

A. Hollfield Tables

2. The January 31, 1984 "Hollfield Tables" indicate that the IRB Fiscal Year 1985 budget request for the URS program totalled $12,700,000, including $12,550,000 for operating expenses and $150,000 for plant and capital equipment (PACE). According to these Tables, the Department's FY 1985 submission to OMB for the program totalled $20,000,000 including $19,850,000 for operating expenses and $150,000 for PACE. What are the specific differences between these two budgets?

Answer:

($ in Thousands)

	FY 1985 IRB Request	FY 1985 OMB Request	Change
University Research Support			
Univ/National Laboratory Cooperative Research			
Operating Expenses.....	$11,750	$11,150	$- 600
Capital Equipment.....	150	150	0
Subtotal.....	11,900	11,300	- 600

	FY 1985 IRB Request	FY 1985 OMB Request	Change
Energy Manpower Development			
Operating Expenses.....	800	700	- 100
Subtotal, URS.....	12,700	12,000	- 700
University Research Instrumentation			
Operating Expenses.....	0*	8,000	+8,000
Total, URS/URI.....	$12,700	$20,000	$+7,300

* The Office of Energy Research submitted a separate request for $10,000,000 in the Internal Review Budget (IRB) for University Research Instrumentation, not included in the URS budget request. The Department decided during IRB deliberations, to include $8,000,000 as part of the OMB request for the URS program.

- The University Research Instrumentation Program was a separate budget submission for the IRB request. This explains the above $8,000,000 increase for this program.

- $700,000 URS difference includes: 1) a reduction of $200,000 in the Reactor Fuel Assistance activity, 2) $200,000 reduction in the Energy Graduate Research Training activity, 3) $200,000 reduction in the Visiting Scientist activity, and 4) a $100,000 reduction in Energy Manpower Assessment activity.

3. **As noted in question 2 above, the Hollfield Tables indicated that the OMB FY 1985 budget request for the URS program totalled $20,000,000, including $19,850,000 for operating expenses and $150,000 for PACE. The FY 1985 Congressional request for URS totalled $9,200,000, all for operating expenses. What are the specific differences between these two budgets?**

Answer:

($ in Thousands)

	FY 1985 OMB Request	FY 1985 Cong. Request	Change
University Research Support			
Univ/National Laboratory Cooperative Research			
Operating Expenses.....	$11,150	$ 8,450	$- 2,700
Capital Equipment.....	150	0	- 150
Subtotal.....	11,300	8,450	- 2,850
Energy Manpower Development			
Operating Expenses.....	700	750	+ 50
Subtotal, URS.....	$12,000	$9,200	$- 2,800
University Research Instrumentation			
Operating Expenses.....	8,000	0*	- 8,000
Total, URS/URI.....	$20,000	$ 9,200	$-10,800

* The OMB requested the Department submit an individual budget request for University Research Instrumentation in the Congressional submission.

- The University Research Instrumentation Program is a separate budget submission in the Congressional Request. This explains the $8,000,000 decrease in the URS program.

- The Energy Graduate Research Training activity, the Visiting Scientist activity, and capital equipment were eliminated.

4. **Given the information in questions 2 and 3 above, what are the specific differences between the Department's FY 1985 IRB and the Congressional Request budgets for URS?**

Answer:

($ in Thousands)

	FY 1985 IRB Request	FY 1985 Cong. Request	Change
University Research Support			
Univ/National Laboratory Cooperative Research			
Operating Expenses.....	$11,750	$ 8,450	$- 3,300
Capital Equipment.....	150	0	- 150
Subtotal.....	11,900	8,450	- 3,450
Energy Manpower Development			
Operating Expenses.....	800	750	- 50
Total, URS.....	$12,700	$9,200	$- 3,500

- In the Congressional Budget Submission three activities were eliminated: 1) the Energy Graduate Research Training activity (3.0M), 2) the Visiting Scientist activity (1.0M), and 3) Capital Equipment (0.2M)

- The Reactor Fuel Assistance activity decreased by 0.1M.

- The University Laboratory Cooperative Research activity increased by 0.8M.

B. University-Laboratory Cooperative Research

5. **How many individuals have participated or are expected to participate in this program for the period FY 1981 - FY 1985? What was the number of participants for each DOE laboratory?**

Answer: Appointments are made for faculty, graduate and undergraduate students to participate in on-going research at a variety of DOE laboratories. Research appointments made in this program since FY 1981 are shown below:

FY 1981	957
FY 1982	1028
FY 1983	1065
FY 1984	1040 (est)
FY 1985	1750 (est)

In addition to the research appointments there are 600 to 700 faculty and students who participate each year in short-term workshops, institutes and conferences on energy-related topics of current interest.

There are eleven contractors currently participating in the Lab Coop program including three university consortia who interface with several laboratory or contractor facilities for the placement of faculty and students. These are Associated Western Universities (AWU), Oak Ridge Associated Universities (ORAU) and the Northwest College and University Association for Science (NORCUS).

Contractor	No. Participants (FY 1983)
Ames Laboratory	29
Argonne National Laboratory	378
Associated Western Universities	169
- Los Alamos National Laboratory	
- Sandia National Laboratories	
- Inhalation Toxicology Research Institute	
- Lawrence Livermore National Laboratory	
- Stanford Linear Accelerator Center	
- Lawrence Berkeley Laboratory	
- Idaho National Engineering Laboratory	
Brookhaven National Laboratory	87
Lawrence Berkeley Laboratory	15
Mound	6

Contractor	No. Participants (FY 1983)
Northwest College and University Association for Science	131
- Boeing Computer Services	
- Hanford Environmental Health Foundation	
- Pacific Northwest Laboratory (Battelle)	
- Rockwell Hanford Operations	
- UNC Nuclear Industries, Inc.	
- Westinghouse Hanford Company	
Oak Ridge Associated Universities	125
- Oak Ridge National Laboratory	
- Atmospheric Turbulence Diffusion Laboratory	
- Center for Energy Environment Research	
- Savannah River Ecology Laboratory	
- Morgantown Energy Technology Center	
Oak Ridge National Laboratory	60
Savannah River Ecology Laboratory	27
Savannah River Laboratory	38

C. University Reactor Fuel Assistance

6. What are Materials Test Reactor (MTR) type fuel elements?

Answer: MTR type elements are Aluminum clad, plate type elements similar to those used in the old Materials Test Reactor in Idaho.

7. How many university research reactors are licensed by the Nuclear Regulatory Commission, and where are they located? How many of these are still operating?

Answer: There are 50 University Research and training reactors and critical facilities (zero power) licensed by the NRC located in 27 states and D.C. Thirteen others have been shut down.

Locations of Currently Licensed Research and Training Reactors

Brigham Young University
Catholic University
Columbia University
Cornell University*
Georgia Institute of Technology*
Idaho State University
Iowa State University
Kansas State University
Manhattan College
Massachusetts Institute of Technology
Memphis State University
Michigan State University
North Carolina State University
Ohio State University
Oregon State University
Pennsylvania State University
Purdue University
Reed College
Rensselaer Polytechnic Institute
Rhode Island Atomic Energy Commission
State University of New York, Buffalo
Texas A&M University*
University of Arizona
University of California, Berkeley
University of California, Irvine
University of California, Los Angeles
University of California, Santa Barbara
University of Florida
University of Illinois*
University of Kansas
University of Lowell
University of Maryland
University of Michigan
University of Missouri, Columbia
University of Missouri, Rolla
University of New Mexico

University of Oklahoma
University of Texas
University of Utah
University of Virginia*
University of Washington
University of Wisconsin
Virginia Polytechnic Institute and State University
Washington State University
Worchester Polytechnic Institute

*Each of the above universities with an asterick has two reactors.

8. **With the exception of fuel assistance, does the DOE provide any funding for any university reactors, and if so, which ones?**

Answer: Yes, funding was provided in the form of reactor sharing grants to seventeen university reactors in FY 1983. This provides for some of the additional costs when the reactor is used by other researchers from other colleges or universities for training and research. Also, some support is provided in the form of services in DOE research contracts, e.g., when materials are irradiated or tested.

University Reactors for FY 1983
University of Florida
Georgia Institute of Technology
Kansas State University
Massachusetts Institute of Technology
University of Maryland
University of Michigan
University of Missouri - Columbia
University of Missouri - Rolla
North Carolina State University
Ohio State University
Oregon State University
Pennsylvania State University
Reed College
Texas A&M University
University of Virginia
University of Wisconsin
Washington State University

Proposals for reactor sharing assistance in FY 1984 have been initiated and are now being submitted. The number and level of grants for FY 1984 are yet to be selected but will be approximately the same as FY 1983.

9. **How many, and which, of the research reactors use highly enriched uranium and which are using the new low enriched uranium fuel?**

Answer: There are 23 university reactors and/or critical facilities using high enriched uranium.

University Research and Training Reactors with HEU Fuel

University/Laboratory	Location
Plate Type Fuel, 93% Enriched Uranium	
High Power	
University of Missouri-Columbia	Columbia, MO
Massachusetts Inst. of Technology	Cambridge, MA
Georgia Inst. of Technology	Atlanta, GA
Medium Power	
Rhode Island Nuclear Science Center	Narragansett, RI
University of Virginia-UVAR	Charlottesville, VA
University of Lowell	Lowell, MA
Low Power	
University of Missouri-Rolla	Rolla, MO
Ohio State University	Columbus, OH
University of Kansas	Lawrence, KA
Worcester Polytechnic Institute	Worcester, MA
Purdue University	West Lafayette, IN
Rensselaer Polytechnic Institute	Troy, NY
University of Virginia-Cavalier	Charlottesville, VA
Manhattan College	Riverdale, NY
TRIGA, UZrH Rod Fuel 70% Enriched Uranium	
Oregon State University	Corvallis, OR
Texas A&M University	College Station, TX
University of Wisconsin	Madison, WI
Washington State University	Pullman, WA
ARGONAUT, Plate Fuel 93% Enriched Uranium	
University of California-Los Angeles	Los Angeles, CA
University of Florida	Gainesville, FL
University of Washington	Seattle, WA
Virginia Polytechnic Institute and State University	Blacksburg, VA
Iowa State University	Ames, IA

The University of Michigan (FNR) is the only reactor using the "new" low enriched uranium fuel. Other reactors are using fuel enriched to less than 20% U-235.

10. **Some concern has been expressed recently that university research reactors which are using highly enriched uranium fuel pose an undue safety and security risk. Does this concern have any validity?**

Answer: None of the University Research Reactors have unirradiated fuel on hand in excess of the five kilogram "formula quantity" rule. This is the amount of special nuclear material, determined by NRC, to be safely below that quantity required to make a critical mass. All university research and training reactors are under NRC safeguard regulations appropriate to their particular facility. These regulations and procedures, as implemented by NRC, are aimed at ensuring that fuel could not be removed by unauthorized parties without detection.

11. **For the University Reactor Fuel Assistance Program, please provide the funding levels and the number and location of university reactors which have, or which are expected to receive assistance for the period FY 1981 - FY 1985.**

Answer: The first table lists costs for fuel fabrication for university research reactors. The different dollar amounts reflect the amount and design of the fuel used. The reactors with higher power levels are in greatest demand for research purposes and thus have longer operating schedules utilizing more fuel.

The second table breaks out the universities receiving reactor sharing grants when they make their facilities and equipment available to researchers and faculty from other institutions.

Reactor Fuel Assistance

	FY 1981	FY 1982	FY 1983*	FY 1984 (est)	FY 1985 (est)
MIT	$ 0	$336K	$ 0	$ 60K	$120K
U. of Missouri	558K	720K	0	348K	300K
U. of Michigan	65K	13K	0	180K	180K
U. of Lowell	0	60K	0	0	60K
R.I. Nuc. Sc. Center	300K	150K	0	0	160K
U. of Virginia	234K	104K	0	78K	180K
Reed College	0	0	8K	0	0

* In FY 1983 there was a change in contractor for fuel fabrication from Atomics International in Canoga Park, CA to Babcock & Wilcox in Lynchburg, VA. The funding was used for the shut down of the AI facility, the transfer of production line equipment to Lynchburg and setting up of the new facility and production line. Therefore the only reactor fueled in FY 1983 was the Triga reactor at Reed College with the fuel provided by General Atomics.

University Reactor Sharing Program

	FY 1981	FY 1982	FY 1983	FY 1984	FY 1985
Univ. of Arizona	$ 0	$ 4,300	$ 0	(To be determined through	
UCLA	0	5,000	0	competitive proposal	
Univ. of Florida	0	0	16,000	selection)	
Georgia Tech.	0	18,000	18,000		
Kansas St. Univ.	4,000	4,000	5,500		
Mass Ins. of Tech.	33,000	35,000	35,000		
Univ. of MD	12,000	13,000	12,000		
Univ. of Michigan	16,000	18,000	18,000		
Univ. of Missouri - Columbia	40,000	45,000	45,000		
Univ. of Missouri - Rolla	0	0	8,000		
SUNY Buffalo	0	0	0		
N.C. State Univ.	5,000	5,000	5,000		
Ohio State Univ.	16,000	15,000	15,000		
Oregon State Univ.	0	0	10,000		
Penn. State Univ.	2,000	2,000	4,800		
Reed College	0	5,000	5,500		
Texas A&M Univ.	20,000	25,000	25,000		
Univ. of Virginia	3,800	4,800	5,500		
Univ. of Wash.	0	9,000	0		
Univ. of Wisconsin	4,300	0	8,500		
Wash. State Univ.	20,000	18,000	15,000		
Total	$176,100	$226,100	$251,800	$250,000	$300,000

12. What would be the cost of refueling all currently operating research reactors with the new low enriched uranium fuel? How long would it take to complete the refueling?

Answer: The cost of refueling including extra costs imposed on the universities for relicensing actions and any facility modifications was estimated by the university study group at about $15M.

The period of time for refueling all university reactors would be in the range of five to six years. This time period is related to the progress of the R&D program developing the alternative low enriched uranium fuel. At this point in time only one type of fuel has been demonstrated, (the 1.6g/cc uranium density for the Mich. reactor). Higher density fuel will be needed for other reactors.* Miniplates of silicide fuel with varying uranium loadings are being tested in U.S. and foreign research reactors to gather the required data.

The Department of Energy recognizes that an orderly change over to the use of low enriched uranium is an appropriate course to follow when the reactor can continue to effectively and safely operate as designed, and the costs of conversion are reasonable.

* Two of the current university reactors (MIT and Missouri) cannot be operated on the low enriched uranium fuel currently under development.

D. Energy Manpower Assessment

13. **Please provide a listing of all completed and ongoing manpower assessments carried out by this program from FY 1981 - present. Please list the performer of each of the assessments and the cost of each.**

Answer: The Energy Manpower Assessment Program has used a variety of contractors and performers to carry out specific manpower assessments. In the last several years, a number of studies have been conducted for the program by both the National Science Foundation (NSF) and the Oak Ridge Associated Universities (ORAU). NSF, through the Science Resources Studies Program, includes energy-related questions in the annual and biennial national surveys of scientists and engineers. ORAU carries out technology specific assessments of the supply and demand of scientific and technical manpower for current and future energy R&D programs. Funds provided by the Energy Manpower Assessment Program to both NSF and ORAU since FY 1981 are totalled below along with the specific reports and assessments produced by each.

National Science Foundation	$360,000
Postcensal National Survey of Scientists and Engineers in Energy Work	200,000
Doctoral Scientists and Engineers in Energy-Related Activities (2 surveys)	45,000
Recent Science and Engineering Graduates Involved in Energy Work (2 surveys)	91,000
Current Labor Conditions for Scientists and Engineers in Energy Industries (2 surveys)	24,000
Oak Ridge Associated Universities	1,072,000
Occupational Employment in Nuclear Energy (2 surveys)	235,000
Nuclear Engineering and Health Physics Enrollments and Degrees (annually)	54,000
Employment and Characteristics of PhDs in Energy Work (2 studies)	48,000
Participation of New BS/MS Graduates in Energy Work (2 studies)	27,000
Development of Annual Energy Manpower Reports Impact of Energy R&D Funding and Production Activities on Science and Engineering Employment Assessment of Adequacy of Supply (3 studies)	460,000
Updating the Data Base of the Total Science and Engineering Population in Energy Work	218,000

Education and Training Implications of Biomass Energy Systems (partial support with other DOE offices)	30,000
National Industrial Conference Board	135,000
Occupational and Training Requirements for Expanded Coal Production	
Department of Labor	30,000
Projections of Cost and Labor Requirements for Constructing Electric Generating Plants (partial support w/other agencies)	
University of Tennessee	90,000
Occupational Requirements for Energy Construction Developments in the U.S. (2 studies)	
University of Utah	94,000
Geothermal Energy Employment and Requirements, 1977-1990	
Kramer Associates, Inc.	79,000
Development of Energy Manpower Factbook	

14. What are the reasons for the large increase (+66.7%) in the Energy Manpower Assessment Program for FY 1985 relative to FY 1984?

Answer: The $270K in the FY84 budget for the Manpower Assessment Program (MAP) primarily supports the continued development and updating of a comprehensive energy manpower data base. The purpose of this data base is to provide us with information on current and trend data on the employment and utilization of scientists and engineers in the research, and operation of various energy sources and programs.

The increased budget requested for FY 1985 ($450K) will enable the MAP to undertake two major activities. First, it will provide the support required to continue the collection and analysis of energy-related scientific and engineering manpower data through NSF-supported surveys (e.g., Ph.D. scientists and engineers in energy R&D and other activities; recent scientists and engineering graduates entering the labor market in energy-related activities). Second, by utilizing the information obtained for the overall energy manpower data base, specific assessments can now be undertaken in various energy areas. For example, because of the shifting trends and activities in the nuclear energy industry, two specific assessments related to nuclear technology developments will be undertaken: an analysis of current occupational employment in nuclear-related activities in private industry and government owned-contractor operated facilities; and, an indepth assessment of manpower supply and demand for selected requirements of the nuclear industry (including the continuing study and analysis of the current

and potential supply of new nuclear engineering and health physics/radiation protection graduates required for research, operations, and health and safety activities). Special analyses of the changing patterns of scientific and technical staffing and mobility and biannual "quick response" surveys of the supply/demand for certain scientific and technical specialists in selected non-nuclear fields would also be carried out as needed.

15. **What specific assessments are planned to be initiated during FY 1984 and FY 1985?**

Annual: In FY 1984:

- Annual survey of enrollments and degrees in nuclear engineering.
- Annual survey of enrollments and degrees in radiation protection and health physics.
- Follow-up survey of a national sample of experienced scientists and engineers identified in the 1982 Postcensal Survey to determine current involvement in energy work.
- Survey of a national sample of new science and engineering graduates to assess number and characteristics of those in energy work.
- Quick response survey of current labor market conditions for critical specialities in energy industries.
- Annual assessment of employment requirements and manpower supply implications of projected trends in energy R&D and production activities.
- Analysis of employment, education and other characteristics of doctoral scientists and engineers in energy work, 1983.

In FY 1985:

- Survey of occupational employment in nuclear energy activities in private industry and government owned-contractor operated labs and facilities.
- Annual survey of enrollments and degrees in nuclear engineering.
- Annual survey of enrollments and degrees in radiation protection and health physics.
- Indepth assessment of manpower supply and demand for selected segments of the nuclear industry.
- Biennial survey of doctoral scientists and engineers in the work-force involved in energy work.
- Special analysis of the changing patterns of scientific and engineering employment related to shifting energy R&D and production activities.

- Quick response surveys of current labor market conditions for critical scientific and engineering specialties in energy industries.

16. **Why does DOE need to support this program, given that similar activities are carried out by the U.S. Department of Labor and by the National Science Foundation?**

Answer: DOE has a legislative responsibility specifically spelled out in the Energy Reorganization Act of 1974 (and incorporated in the Department of Energy Organization Act of 1977) to help "assure an adequate supply of manpower for the accomplishment of energy research and development programs... by assuring the collection, analysis and dissemination of necessary manpower supply and demand data."

Although both the Department of Labor and the National Science Foundation carry out activities similar to the manpower assessment programs, neither agency has a mandate or a programmmatic interest in supporting studies in specific mission areas (i.e., defense, energy, health, etc.). It is only because DOE has developed a comprehensive energy manpower data base, specifically keyed to a variety of energy technology areas, that the agency has been able to meet various legislative responsibilities in past years (e.g., in areas of nuclear safety research and development, fusion energy, fossil energy). Also, because these assessments are related to specific energy areas, we have been able to provide data to various DOE program areas in developing their long-range program plans and in dealing with manpower training and development.

If DOE were unable to continue conducting these assessments, then both funds and additional personnel slots would have to be alloted to either NSF or Labor to perform the analyses, synthesis and dissemination of enegy manpower supply and demand studies required under the referenced legislation. Further, the expertise now extant among DOE staff does not exist elsewhere and would be difficult to replicate by the simple addition of new staff in another agency.

Finally, separation of the manpower assessment function from the energy R&D programs in DOE would lead to duplication of effort, increased costs and perhaps increasingly non-useful assessment studies.

E. Energy Education and Training

17. When were the Prefreshman Engineering Program Projects (PREP) initiated and what have been the funding levels since their initiation?

Answer: The purpose of PREP is to encourage additional numbers of women and minority high school students to pursue engineering as an academic and professional career. PREP projects are carried out by local colleges and universities. Substantial local industrial support (over $12 million since 1973) is also provided in addition to the funding from DOE (shown in the table below). PREP was started by the Atomic Energy Commission in 1973. The funding levels by fiscal year are as follows:

FY 1973	- $47,900
FY 1974	- $50,600
FY 1975	- $84,500
FY 1976	- $100,500
FY 1977	- $135,000
FY 1978	- $225,000
FY 1979	- $292,000
FY 1980	- $392,000
FY 1981	- $430,000
FY 1982	- $220,000
FY 1983	- $220,000
FY 1984	- $200,000

18. How many PREP awards have been made since its initiation? What are a few examples of the types of projects that have been supported?

Answer: 156 projects have been supported since the initiation of the program. The number of projects supported each year is as follows:

FY 1973 - 4	FY 1979 - 20
FY 1974 - 4	FY 1980 - 28
FY 1975 - 5	FY 1981 - 26
FY 1976 - 5	FY 1982 - 15
FY 1977 - 4	FY 1983 - 15
FY 1978 - 1	FY 1984 - 14

Several examples of current PREP projects are summarized as follows:

Temple University, Philadelphia, PA

The PREP program at Temple is the first of a series of four summer programs involving four different universities, including Temple, in the Philadelphia area: 8th grade, Temple University, (Mathematics); 9th grade, University of Pennsylvania, (Communications); 10th grade, Drexel University, (Engineering Sciences); and 11th grade, Villanova University, (Engineering Design). During the ten-year history of this project, two-thirds of the participants who started the four year sequence have completed the program. Of these, 86% go on to college, and 92% of these are pursuing engineering.

During the summer of 1983, 80 eighth grade students from 30 different junior high schools attended the four-week program. The selection criteria used were: recommendations from junior high and middle school counselors; score of at least 70% on the California Achievement Tests; a mid-year grade average of 3.0 in math and science; exhibited interest in science and engineering; commitment to attend sessions for four consecutive summers; and parental approval.

A math test is administered to all participants at the beginning of the program. Participants are then divided into four groups based on the test results and the level of instruction is adjusted to fit each group. The major elements of the curriculum are mathematics, advanced mathematics, communications, computer science, advanced computer science (FORTRAN) and engineering. Two field trips to local industries to witness engineers in their working environments are also provided. Homework assignments are made by the staff and completed by the students.

University of Texas - San Antonio

The 1983 San Antonio PREP was conducted on the campus of the University of Texas - San Antonio from June 6 to July 29, 1983. 297 program participants were hispanic high school and middle school students from the various independent school districts of the San Antonio area.

All participants were identified as high ability students and were expected to pursue a demanding college-level schedule for five hours a day, for eight weeks. The academic component of the program included logic and its application to mathematics, introduction to engineering, mathematics, problem solving seminars, presentations by visiting scientists and engineers, field trips to high technology facilities and practice SAT examinations. Since the program started on 1979, 620 students have successfully completed the program; over 70% of college bound students pursue engineering and science studies.

Indiana University - Purdue University at Indianapolis

PREP is a part of the larger, 8-year, Minority Engineering Advancement Program, (MEAP). In the summer of 1983, 137 students in grades 9-12 took part in a two week workshop at Purdue University. The academic program was divided into the following levels:

Level 1

Students who were at the 9-10th grade level participated in an intensive introduction to civil, electrical, and mechanical engineering, as well as computer technology. The introductory work was divided between academic instruction and hands-on application. The students were engaged in 50 contact hours of lectures and laboratory instruction. In the computer sessions, for example, the students worked at computer terminals and learned to program in BASIC.

Level II

Students who are at the 10-11th grade level were involved in two weeks of more intensive work in the four specific areas of engineering covered in Level I.

Level III

At the 11-12th grade level students participated in a two-week schedule of college and employment preparatory workshops that were designed to strengthen basic college-level survival skills and to acquaint students with post-high school and career information, including tours of local industries. A total of 42 hours in lecture and laboratory were given to these participants. Topics covered at this level included: resume preparation, job seeking skills, study skills, motivation and personal growth, and college financial resources. Nine field trips were made to local industry.

Level IV

Fourth year students, who plan to begin engineering collegiate study, interviewed with and joined industrial companies which give additional support to the PREP program for summer intern co-op work experiences. There were eight students employed at this level during the summer of 1983.

Follow-up studies show that over 96% of the students who completed the MEAP program during the last four years entered college. Over 65% chose an engineering or technical discipline of study.

IV. UNIVERSITY RESEARCH INSTRUMENTATION (URI)

1. What is the documented shortage of research equipment in universities?

Answer: The most recent major studies which have documented the shortage of research equipment in universities are:

a. "Revitilizing Laboratory Instrumentation," Report of a workshop of the National Research Council, March 1982.

b. "Scientific Instrumentation Needs of Research Universities," Association of American Universities, (AAU) June 1980.

The overall sense of these reports is that universities are experiencing difficulty undertaking advanced research because many scientific instruments are old, obsolete, and require an excessive amount of funds and time for maintenance. For example, the AAU study estimates that the median age of university research instrumentation was twice that of equipment in comparable commercial laboratories. The AAU report estimates that the total replacement costs of university instrumentation required in science and engineering is about $1 billion to $2 billion. The need for new state-of-the-art energy-related research instrumentation in universities is estimated to be between $100 million to $200 million, or about 10% of the total national need.

2. The January 31, 1984 "Hollifield Tables" indicate that the IRB Fiscal Year 1985 budget request for the URI program totalled $10,000,000 for operating expenses. According to these Tables, the Department's FY 1985 submission to OMB did not contain any funding for the program. Is this correct, and if so, why was the Department willing to abandon the program after only one year?

Answer:

($ In Thousands)

	FY 1985 IRB Request	FY 1985 OMB Request	FY 1985 Cong. Request
University Research Instrumentation			
Operating Expenses.....	$10,000	$ 0*	$ 6,000
University Research Support			
Operating Expenses			
Univ/National Laboratory			
Cooperative Research.....	11,750	11,150	8,450
Energy Manpower Development.....	800	700	750
University Research			
Instrumentation.....	0	8,000*	0
Total Operating Expenses.....	12,550	19,850	9,200
Capital Equipment.....	150	150	0
Total.....	$12,700	$20,000	$ 9,200

* The Department submitted a request for $8,000,000 in the OMB Submission under the University Research Support program, as shown in the table above.

- The difference between the IRB ($10,000,000) and the OMB ($8,000,000) request is approximately 10 instrumentation awards.

- The difference between the OMB ($8,000,000) and the Congressional Submission ($6,000,000) is approximately 10 instrumentation awards.

3. **How many URI awards does DOE expect to make with its $4.0 million in FY 1984, and how many are expected in FY 1985 at the $6.0 million request level?**

Answer: In FY 1984, DOE expects to make about 10-15 awards, totalling $4 million. The $6 million requested for the URI program in FY 1985 will permit the Department to make about 15-20 awards.

4. **What universities are eligible to participate in the program?**

Answer: In order to participate in the Department's University Research Instrumentation (URI) Program an institution must have received $150,000 from DOE for research in a specific, energy-related area (e.g., combustion, bioconversion processes, nuclear waste isolation research, etc.) during the period January 1982 to December 1983. Since the average DOE award to universities for research is about $75,000 per year, an institution need only have the equivalent of one such award for two years to be eligible for the program. It is estimated that 100 to 150 graduate-level research universities and colleges meet this criterion.

5. **What types of instrumentation were supported by DOE in FY 1984, and what types are expected to be supported in FY 1985?**

Answer: The objective of this program is to assist universities and colleges to strengthen their capabilities to conduct long-range energy research by helping them to obtain large, state-of-the-art research instruments which are required for advanced research. Such instruments generally cost between $100,000 and $500,000 each. In FY 1984, DOE will assist universities and colleges to obtain a variety of spectrometers (e.g., mass, nuclear magnetic resonance, infrared Fourier transform, and coherent Raman spectrometers), scanning transmission electron microscopes and electron microprobes, laser analyses systems, and x-ray diffraction equipment. The vast majority of the instruments requested are required for the detection of trace amounts of reaction products and of short-lived chemical species so that we may expand our understanding of energy-related processes. We expect to assist universities to obtain similar types of instrumentation in FY 1985 because these and related analytical instruments are essential for increasing our understanding of all energy-related processes.

6. **How are areas of intrumentation support chosen? What criteria are used?**

Answer: While instrumentation required in all areas of energy research was eligible for support in FY 1984, the URI program placed special emphasis on the equipment needs of four research areas: bioconversion, combustion, nuclear waste isolation research, and turbulence and multiphase flow. These areas were selected after discussions with the Department's senior research staff regarding the topics they felt were of national interest, encompassed

the agency's concerns both with respect to its basic and technology research programs, whose research could benefit substantially from new instrumentation, and which were of interest to researchers in a variety of disciplines. The above areas involve chemists, engineers, biologists, earth, materials and environmental scientists, etc. The areas which will be selected for emphasis in FY 1985 will be chosen after similar discussions with the Department's senior research staff.

7. **What criteria are used in the review and evaluation of the URI proposals?**

Answer: The criteria used in the review and evaluation of proposals are:

a. Technical merit and accomplishments of the institution's research program in the selected energy area; the institution's capability and commitment to energy research in this area, and the potential for expanding/improving the program with the acquisition of the requested equipment.

b. Qualifications of the faculty associated with the applicable research area(s).

c. The institution's plans for cost-sharing (including initial purchase costs, operation and maintenance) of the equipment with non-Federal funds.

d. The institution's experience in utilizing other major research instruments and its plans for enabling faculty at other institutions to utilize it for research.

8. **Who are the members of the Interagency Working Group on Research Instrumentation? How often does it meet, and what is the role of the DOE and each of the other agencies involved in the Working Group?**

Answer: The Interagency Working Group on University Research Instrumentation was established in 1981 by the President's Science Advisor, Dr. George Keyworth, to develop a coordinated government-wide approach towards dealing with the increasing lack of direct access by university scientists to state-of-the-art scientific research instrumentation. The Working Group includes senior level representation (Assistant Secretary or equivalent) from the following agencies concerned with university research: DOD, NASA, NIH, Agriculture, NSF and DOE. The Deputy Director of NSF chairs the Working Group. Five meetings of the Working Group have been held since 1981. Major accomplishments have included the documentation, agency by agency, of university instrumentation needs in specific research areas and the coordination of agency plans towards supporting instrumentation porograms. The Department of Defense was the first agency to develop and implement a special program directed at university research instrumentation needs ($30M in FY 1983 and subsequent budget years). It is focused on defense, science and engineering-related areas. In FY 1984, DOE established a similar instrumentation program ($4M) to help universities to strengthen their energy research programs. Other agencies have increased their support for university research instrumentation as part of their ongoing research programs. In all cases, the Working Group was involved in reviewing and coordinating agency plans and programs related to university research instrumentation. This coordination has proved to be extremely useful to us in the development of our own program. Staff at DOD and NSF assisted us in the development of our program solicitation. We will be coordinating the selection of proposals in our FY 1984 progam with DOD, NSF and other agencies which are providing funds to universities for major research instrumentation.

V. ADVISORY AND OVERSIGHT PROGRAM DIRECTION

1. **What is the actual and estimated funding for this program for the period FY 1981 - FY 1985?**

Answer:

	FY 1981 Actual	FY 1982 Actual	FY 1983 Actual	FY 1984 Estimate	FY 1985 Estimate
Operating Expenses (BA in thousands)	$2,900	$2,925	$2,603	$3,400	$2,900

2. **What are the actual and estimated staffing levels of this program for the period FY 1984 - FY 1985?**

Answer:

	FY 1984 Estimate	FY 1985 Estimate
Full-Time Equivalents	44	44

3. **For the period, FY 1981 - present, what "benefit studies of the results of research programs, evaluations of research that crosscuts programs for integration of objectives and approaches, and independent peer reviews of technical or research subjects as directed by the Secretary or other top management officials" have been performed? What are anticipated for the remainder of FY 1984 - FY 1985?**

Answer: The terms "benefit studies of the results of research programs, evaluations of research that crosscuts programs for integration of objectives and approaches, and independent peer reviews of technical or research subjects as directed by the Secretary or other top management officials" are descriptive of the type of studies undertaken or supported by personnel funded under the Office of Program Analysis. In response to Question 2 of Section II, Energy Research Analysis, a complete listing of the studies performed since FY 1981 and planned for FY 1984 - FY 1985 was provided. A copy is attached.

ATTACHMENT 1

OFFICE OF PROGRAM ANALYSIS (OPA)
PROGRAM AND TECHNICAL ASSESSMENTS
($ IN THOUSANDS)

FY 1981 Obligations

A. Program Assessments

- Assessment of the Office of Health and Environmental Research Program (OPA Staff) (1)..... $ 551

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(1) In each case that OPA Staff is listed, this staff is directly responsible for preparing a technical report; but, typically, Oak Ridge National Laboratory, Los Alamos National Lboratory, or other technical support may have been contracted for assistance.

- Topical Reviews: The Physics and Chemistry of Acid Precipitation; Assessment of Some Energy Technologies Associated with Solar Energy; Climatic Effects of Minor Atmospheric Constituents (SRI-JASON)..... $ 200
- Review of the Advanced Technology Projects for Continuation (OPA Staff)..... -
- Review of MHD Planned Program (OPA Staff)..... -

B. Technical Assessments

- Technology Base Review, DOE R&D Programs (OPA) Staff..... $ 595
- R&D Needs in Coal Liquefaction (University of California/San Diego, Fossil Energy Research Working Group)..... $ 70
- Research Needs in Coal Utilization and Synthetic Fuels Production (American Physical Society)..... $ 10
- Assessment of Factors Affecting Potential of Ethanol as a Transportation Fuel (OPA Staff)..... $ 20
- Assessment of Biomass and Algae (Ecoenergetics, Inc.)..... $ 30
- Assessment of Shale Beneficiation (Massachusetts Institute of Technology)..... $ 88
- Review of Foreign Technology Photosynthetic Production of Fuels and Chemicals (Lawrence Livermore National Laboratory)..... $ 45
- Review of Acid Rain Research (West Point Military Academy)..... $ 15
- Assessment of Liquid Air Engines (R&D Associates)..... $ 100
- Future Availability of Catalyst Metals (Midwest Research)..... $ 54
- Food Chain/Energy Studies (Washington University/St. Louis)..... $ 129
- Energy Research Advisory Board (Los Alamos National Laboratory and Koba Associates)..... $ 590

Total FY 1981 Obligations..... $2,497

FY 1982 Obligations:

A. Program Assessments

- Peer Review and Assessment, Basic Energy Science Program (OPA Staff)..... $ 355
- Assessment of Adequacy of Energy Research Reactor Safety Activities (OPA Staff)..... $ -

- Seminar on Acid Precipitation (General Research Corporation).... $ 14
- Assessment of Electrochemical Storage Program (OPA Staff)..... $ -
- Review and Coordination of Review Comments, Draft National Acid Precipitation Assessment Plan (OPA Staff)..... $ -
- Research Needs Methodology/Procurement Study (OPA Staff)..... $ 5
- Assessments of the Office of Health and Environmental Research's Accomplishments (OPA Staff)..... $ 310
- Interagency Task Force on Acid Precipitation (National Laboratory Consortium)..... $ 25
- An Operational Research Plan for Acid Precipitation (National Laboratory Consortium)..... $ 200

B. Technical Assessments

- Assessment of Research Needs in Energy Conversion and Conservation (Research and Management Technicians, Inc.)..... $ 100
- Assessment of the Office of Health and Environmental Research's Nuclear Instrumentation Accomplishments (Ecosometrics, Inc.).... $ 58
- Assessment of the Office of Health and Environmental Research's Environmental and Health Indentification and Evaluation Accomplishments (SRA Corporation)..... $ 60
- Assessment of Research Needs for Geothermal Energy (Engineering and Economics Research)..... $ 50
- Review and Commentary on Paper Drafted by the United States/Canada Coordinating Committee on Transboundary Air Pollution (OPA Staff)..... $ -
- Assessment of Research Needs in Nuclear Waste (Southern Science Applications, Inc.)..... $ 100
- Topical Reviews: Heavy Ion Fusion; Overview of the Physical-Chemical Processes in the Formation of Acid Precipitation; CO_2 and Climate; Production of Nuclear Material (JASON)..... $ 200
- Assessment of Research Needs in Solar Thermal (TPI, Inc.)..... $ 74
- Methanol and Ethanol as Alternative Fuels for Automotive Piston Engines (OPA Staff)..... $ -
- Assessment of Research Needs in Photovoltaics (DHR, Inc.)..... $ 86
- Assessment of Coal Combustion (Coal Combustion Applications Working Group, University of California)..... $ 88

- Acid Precipitation Research Assessment Support (West Point Military Academy)..... $ 50
- Technology Base Assessments, DOE R&D Programs (OPA Staff)..... $ 428
- Assessment of Research Needs in Drilling and Other Assessment Assistance (Oak Ridge National Laboratory and Sandia National Laboratories)..... $ 75
- Energy Research Advisory Board (Oak Ridge National Laboratory and Koba Associates)..... $ 549

Total FY 1982 Obligations..... $2,847

FY 1983 Obligations

A. Program Assessments

- Assessment of Major Accomplishments of the Office of Health and Environmental Research (OPA Staff)..... $ 75
- Preparation and Coordination of Input to Annual Science and Technology Report to Congress (OPA Staff)..... $ -
- Interagency Task Force on Acid Precipitation (OPA Staff)..... $ 44
- Preparation and Coordination of Executive Summary and Other Parts of the Interagency Task Force on Acid Precipitation's Annual Report (OPA Staff)..... $ -
- Commentary on "National Strategy for Fast Breeder Reactor Development" (OPA Staff)..... $ -
- DOE Input to the International Energy Agency's Annual Report on Energy R&D (OPA Staff)..... $ -
- International Energy Agency's Energy Technology Studies (Brookhaven National Laboratory)..... $ 12
- Peer Review and Assessment of Research Programs in Enhanced Oil and Gas Recovery (OPA Staff)..... $ 165
- Assessment of DOE Position on Private Ownership of Civil Land Remote Systems (OPA Staff)..... $ -
- Peer Review and Assessment of Solar Research Projects at the National Bureau of Standards (OPA Staff)..... $ 60
- Peer Review and Assessment of Conservation Projects at the National Bureau of Standards (OPA Staff)..... $ -
- Assessment of Report by Donald Rice, Rand Corporation, on Need for Clinch River Breeder Reactor (OPA Staff)..... $ -

B. Technical Assessments

- Interagency Memorandum of Understanding with the Environmental Protection Agency on Acid Precipitation (Brookhaven National Laboratory)..... $ 520
- Acid Precipitation Research Assessment Support (West Point Military Academy)..... $ 15
- Battery Technology Transfer (Argonne National Laboratory)..... $ 125
- Risk Analysis - Atmospheric Dispersion from Acid Rain (Brookhaven National Laboratory)..... $ 80
- Risk Analysis - Liquid Metal Fast Breeder Reactor (Oak Ridge National Laboratory)..... $ 125
- Acid Rain Transport Experiment Support Proposed by the Tennessee Valley Authority (Oak Ridge National Laboratory)..... $ 23
- Drilling Research Assessment (Oak Ridge National Laboratory and Sandia National Laboratories)..... $ 52
- Modeling Symposium - Acid Rain (Oak Ridge National Laboratory).. $ 50
- Assessment of Coal Combustion Long-Range Research (Coal Combustion Applications Working Group, University of California)..... $ 11
- Topical Reviews: Acid Rain; Tailored Nuclear Weapons; Photovoltaics; Muon Catalyzed Fusion (JASON)..... $ 200
- Assessment of Research Needs in Photovoltaics (DHR, Inc.)..... $ 27
- Assessment of Research Needs in Energy Conversion and Conservation (Research and Management Technicians, Inc.)..... $ 10
- Assessment of Current Status and the Potential of Alternate Power Reactor Concepts (OPA Staff)..... $ -
- Reviews of Technology Development Histories for the International Energy Agency's Energy Technology Policy Study (OPA Staff)..... $ -
- Reviews of Foreign Technology (Foreign Applied Sciences Assessment Center)..... $ 140
- Energy Research Advisory Board (Oak Ridge National Laboratory and Koba Associates)..... $ 613
- Assessment of Needs in Continental Scientific Drilling (Columbia University)..... $ 98
- Assessment of Factors Influencing Public Perceptions of Energy Systems Deployment (DuPont Associates)..... $ 87

- Acid Rain Research and Other Assessment Support to OPA Staff (Oak Ridge National Laboratory)..... $ 291

Total FY 1983 Obligations..... $2,823

FY 1984 and FY 1985 Estimates:

A. Program Assessments

- Assessment of Extent to Which Research Recommendations of Prior Review Panels in Fossil Energy Have Been Carried Out (OPA and Fossil Energy Staff)..... $ -
- Assessment of Need for Continuation of High Altitude Sampling Program in the Office of Health and Environmental Research (OPA Staff)..... $ -
- Assessment of the Advanced Research and Technology Development Projects in Fossil Energy (OPA Staff)..... $ 400

B. Technical Assessments

- Assessment of Research Needs in Drilling (Oak Ridge National Laboratory and Sandia National Laboratories)..... $ 64
- Atmospheric Studies and Other Research Needs (JASON)..... $ 400
- Assessment of Four Solar Technologies for H_2 Production (Solar Energy Research Institute)..... $ 100
- Assessment of Research Needs in Large-Scale Systems (Carnegie-Mellon University)..... $ 53
- Assessment of Fuel Cell Research (University of California, Advanced Fuel Cell Working Group)..... $ 129
- Reviews of Foreign Technology (Foreign Applied Sciences Assessment Center)..... $ 280
- Assessment of Research Needs in Acid Precipitation (Brookhaven National Laboratory, Oak Ridge National Laboratory and Pacific Northwest Laboratory)..... $1,047
- Support of Interagency Task Force on Acid Rain (OPA Staff)..... $ 87
- Assessment of Technology Status: International Energy Agency (Department of Energy, International Energy Agency, and Brookhaven National Laboratory)..... $ 52
- Assessment of Bioengineering and Bioconversion Energy Research Needs (Under Request for Proposals)..... $ 125
- Assessment of Wind Energy Research Needs (Under Request for Proposals)..... $ 125

- Assessment of Nonhighway Transportation Research Needs (Under Request for Proposals)..... $ 125
- Assessment of Materials Research Needs for Advanced Energy Technologies (Under Request for Proposals)..... $ 125
- Interagency Memorandum of Understanding with the Environmental Protection Agency on Acid Precipitation (Oak Ridge National Laboratory)..... $ 240
- Improved PWR Fuel (OPA Staff)..... $ 6
- Program and Technical Assessment Support (National Laboratories and Others)..... $1,311
- Energy Research Advisory Board (Oak Ridge National Laboratory and Others)..... $1,200

Total FY 1984 and FY 1985 Estimated Obligations..... $5,869

4. **How many consultants has this program used for the period FY 1981 - present? Who were these consultants, what services did they perform, and what fees were paid?**

Answer: This program has utilized two consultants from FY 1981 to the present. Data on these individuals and their associated costs follow:

	FY 1981	FY 1982	FY 1983	FY 1984
Robert C. Stephenson	$14,653	$15,781	$ 6,973	0

Mr. Stephenson was employed on an intermittent basis to provide expert advice on the development of information on DOE/university R&D program opportunities, to advise on the impact of DOE/university procurement/assistance regulations, and to provide technical advice on proposal review and evaluation criteria in the university research program. His appointment was not renewed for FY 1984.

	FY 1982	FY 1983
Norman H. Kreisman	$19,691	$39,956

Mr. Kreisman was employed for one year as a temporary expert to assist in establishment of a technology transfer program for the DOE laboratories and to assist in institutional planning for efficient utilization of the program laboratories. He was subsequently converted to a full-time permanent employee.

5. **What is the Laboratory Management Council? Who are its current members, and what level of funding has the Council received and is estimated to receive for the period FY 1981 - FY 1985?**

Answer: The Laboratory Management Council, which supersedes the Field and Laboratory Coordination Council, was established by the Secretary on September 22, 1983. The Council consists of the programmatic officials responsible for research and development activities taking place at the laboratories

which are under the Department's cognizance. It reviews significant issues and policy questions pertaining to the utilization and management of these laboratories.

Specifically, the Chairperson is the Special Assistant to the Secretary. The Council includes as its members the Director of Energy Research and the Assistant Secretaries for Defense Programs, Nuclear Energy, Fossil Energy, Conservation and Renewable Energy, and Management and Administration. Additional Headquarters officials are invited on a case-by-case basis depending on agenda items.

There is no funding for the Council.

6. **Who are the current members of the Energy Research Advisory Board (ERAB), and what level of funding has ERAB received and is estimated to receive for the period FY 1981 - FY 1985?**

Answer: A list of the current ERAB members and their organizational affiliations is attached. As required by the ERAB charter, the Department is currently in the process of selecting approximately 8-10 new members to replace current members whose terms are ending.

The Department provides funds to ERAB and its panels for travel expenses and for analytic studies and research required in order to carry out their studies. The funds, which support the Board and an average of three to four panels in each fiscal year, have been essentially level at $670-680 thousand in FY 1981 through FY 1984, and are expected to be about the same in FY 1985. Of this amount, only $80,000 for the travel expenses of the ERAB itself and the Headquarters support staff is provided from Advisory and Oversight Program Direction. The balance is provided by the Energy Research Analysis program and includes $100,000 for travel expenses of the panel members.

ENERGY RESEARCH ADVISORY BOARD

Louis H. Roddis, Jr., P E.
Consulting Engineer
Charleston, SC

Betsy Ancker-Johnson
Vice President
Environmental Activities Staff
General Motors

Frank P. Baranowski
Great Falls, VA

Ivan L. Bennett
Professor of Medicine
New York University Medical Center

Solomon J. Buchsbaum
Executive Vice President
Bell Laboratories

Melvin Calvin
Professor of Chemistry
Department of Chemistry
University of California

William D. Carey
Executive Officer
American Association for the Advancement of Science

Charles F. Cook
Vice President Research and General Development
Phillips Petroleum Company

Floyd L. Culler, Jr.
President
Electric Power Research Institute

Gerald L. Decker
President and Chief Executive Officer
Decker Energy International, Inc.

John S. Foster, Jr.
Vice President for Science and Technology
TRW, Inc.

Robert L. Hirsch
Vice President, Exploration and Production Research
ARCO Oil & Gas Co.

Charles J. Hitch
President Emeritus
University of California

Henry R. Linden
President
Gas Research Institute

William T. McCormick, Jr.
President
American Natural Resources Company

Laurence I. Moss
Estes Park, Co.

David Pimentel
College of Agriculture
Cornell University

Robert H. Pry
Consultant
Gould, Inc.

Eric Reichl
President (Retired)
Conoco Coal Development Company

Alan Schriesheim
Sr. Deputy Director
Argonne National Laboratory

John W. Simpson
Consultant to International Energy Associates

Clifford V. Smith, Jr.
Special Assistant to the Chancellor and Director of CASEERI
Portland State University

Grant P. Thompson
Senior Associate
The Conservation Foundation

Victoria J. Tschinkel
Secretary
Department of Environmental Regulation
State of Florida

STAFF:
Thomas J. Kuehn, Executive Director
Energy Research Advisory Board
U.S. Department of Energy
1000 Independence Avenue, SW.
Washington, D.C. 20585
Tel. 202/252-8933

7. **What is the Field Management Board? Who are its current members, and what level of funding has the Board received and is estimated to receive for the period FY 1981 - FY 1985?**

Answer: The Field Management Board does not exist at DOE; it was one of the names considered by DOE for what is now the Laboratory Management Council, discussed in Question 5 above.

8. **For which five Energy Research multiprogram laboratories does the Advisory and Oversight Program Direction staff prepare institutional plans? Why don't these laboratories prepare their own plans?**

Answer: The statement in the budget request that "staff will continue to prepare institutional plans..." is badly worded. The staff has never prepared plans for the laboratories. The laboratories prepare their own plans. The staff provides annual instructions for the preparation of these plans and reviews the plans of all the laboratories.

A. Hollfield Tables

9. The January 31, 1984 "Hollfield Tables" indicate that the IRB Fiscal Year 1985 budget request for Advisory and Oversight Program Direction totalled $4,700,000, for operating expenses. According to these Tables, the Department's FY 1985 submission to OMB for this totalled $3,450,000 for operating expenses. What are the specific differences between these two budgets?

Answer: The FY 1985 IRB request for Advisory and Oversight Program Direction was $4,700,000 compared to the OMB request of $3,450,000, a difference of $1,250,000. This line is for salaries, benefits, and associated staff support costs.

- The difference between the two budgets is a reduction of 22 full-time equivalents (FTE's), from 69 FTE's in the IRB request to 47 FTE's in the submission to OMB.
- Of the total difference, the IRB request for 12 FTE's and associated costs of $750,000 to carry out the Energy Science Computational Research (ESCR) function was revised and submitted to OMB as part of the ESCR decision unit.
- The remaining difference of $500,000 was associated with elimination of 10 FTE's which were requested to support the Field Operations Management, University Research Support, and Energy Research Analysis activities.

10. As noted in question 9 above, the Hollfield Tables indicated that the IRB FY 1985 budget request for the Advisory and Oversight Program Direction totalled $4,700,000, for operating expenses. The FY 1985 Congressional request for this totalled $2,900,000 for operating expenses. What are the specific differences between these two budgets?

Answer: The FY 1985 IRB request for Advisory and Oversight Program Direction was $4,700,000 compared to the Congressional request of $2,900,000, a difference of $1,800,000.

- The difference between these two budgets is a reduction of 25 FTE's from 69 FTE's in the IRB request to 44 FTE's in the Congressional request.
- Twelve FTE's and $750,000 associated with Energy Science Computational Research (now Applied Mathematical Sciences subprogram in Basic Energy Sciences) were eliminated from Advisory and Oversight Program Direction.
- Thirteen FTE's requested to support the Field Operations Management, University Research Support, and Energy Research Analysis activities were eliminated, resulting in a reduction of approximately $900,000.
- The remaining difference of $150,000 reflects miscellaneous savings to be achieved through a change in the personnel mix resulting in a reduction in average salary as well as reductions in other compensation requirements.

11. Given the information in questions 9 and 10 above, what are the specific differences between the Department's FY 1985 submission to OMB and the Congressional Request budgets for Advisory and Oversight Program Direction?

Answer: The FY 1985 OMB request for Advisory and Oversight Program Direction was $3,450,000 compared to the Congressional request of $2,900,000, a difference of $550,000.

- The difference between these two budgets is a reduction of 3 FTE's from 47 FTE's in the OMB request to 44 FTE's in the Congressional request.

- Of the total difference, $400,000 is related to the reduction of 3 FTE's requested to support the Field Operations Management and University Research Support activities, and to reflect a funding reduction consistent with the total FTE reduction from the original IRB request.

- The remaining difference of $150,000 reflects miscellaneous savings to be achieved through a change in the personnel mix resulting in a reduction in average salary as well as reductions in other compensation requirements.

B. Laboratory Appraisal Process

12. Who performs laboratory appraisals?

Answer: Appraisals are performed by Headquarters and field elements depending on the nature and scope of the area being examined. In order to establish a uniform and systematic approach for appraising performance of the DOE multiprogram laboratories, an order was issued October 6, 1983, setting forth DOE policy and guidance for the appraisal of those laboratories. Under this order, Operations Office Managers are responsible for conducting an annual overall appraisal of the laboratory. This overall appraisal incorporates the results of all individual appraisals conducted during the year.

13. What is involved in the current laboratory appraisal process? Are laboratories appraised on a program-by-program basis?

Answer: The Operations Office Managers, as contract officers, develop an annual appraisal plan tailored to recognize specific characteristics of each multiprogram laboratory under their purview. The plan includes critical areas of performance and appraisal criteria and, after being submitted to the cognizant Secretarial Officer for review, is provided to the laboratory at the start of the appraisal period. An annual written summary appraisal report on findings and recommendations for activities evaluated is prepared by the Operations Office and is provided to the laboratory director for appropriate action. Laboratory response to the appraisal is reported to the cognizant Secretarial Officer as part of the annual Institutional Planning on-site review.

One of the overall appraisal areas considered by the Operations Office Manager is program performance which evaluates programs at the laboratories in terms of quality of scientific and technical performance and achievements. Not all programs at the laboratory are evaluated each year but are covered over a three year period.

14. What specific measures of effectiveness and performance criteria are used to appraise the laboratories? What are the weightings given each of these measures of effectiveness and performance criteria?

Answer: Appraisal plans include critical areas of performance and appraisal criteria and are tailored to the specific characteristics of each multiprogram laboratory. Appraisals are in four broad areas of performance: management, programs, operations support, and administration. Within each of these broad areas are more specific items for which effectiveness and performance are evaluated. In programmatic performance, for example, the laboratory may be judged on the efficacy of its program and project planning, its effectiveness in meeting program objectives, achievements in research and development, the quality and quantity of scientific work, appropriate reporting of accomplishments, and adherence to technical, cost and schedule milestones.

While qualitative judgements are given for each item being appraised, there are no weightings, per se, assigned to them. One of the objectives of the appraisal system is to identify deficiencies and areas needing improvement and to assure that corrective actions are taken. It also recognizes the laboratory for those areas where performance has been outstanding or superior.

15. What changes are expected to be made in the appraisal process?

Answer: The DOE order covering the appraisal of multiprogram laboratory performance was issued on October 6, 1983, and there has not yet been sufficient experience to determine whether any changes will be necessary. The Director of the Office of Energy Research has the responsibility for the periodic review of the appraisal policy and its implementation. He has been closely following the implementation of the appraisal order and will make his report, including recommendations, after the completion of the FY 1984 appraisal cycle.

C. ERAB Multiprogram Laboratory Panel September 1982 Recommendations

1.0 Appropriate Roles and Missions of the Laboratories Vis-a-Vis Universities and Industry

16. What is being done to implement the September 1982 ERAB report's recommendations on the appropriate role and missions of the laboratories vis-a-vis universities and industry?

Answer: As part of the institutional planning process Secretary Hodel issued the Department's policy guidance on the role and missions of the multiprogram laboratories. The Secretary's policy guidance is based on his Congressional statement on the Federal role in energy R&D, and is consistent with the National Energy Policy Plan. The Laboratory Management Council (LMC) developed a general laboratory role statement and reviewed all proposed laboratory mission statements.

2.0 Scientific and Technological Capabilities of the Laboratories

17. What is being done to implement the recommendation that the DOE "Urge the Office of Management and Budget to support rolling two-year appropriations by Congress for research and development with carry over funding to stabilize the Department and laboratory planning and program execution"?

Answer: The Secretary has supported this recommendation in meetings with laboratory directors, OSTP and Congress.

DOE support was also noted in the Director of Energy Research's December 2, 1982 testimony.

18. What is being done to implement the recommendation that DOE "Designate a high level official, such as a Deputy Undersecretary, whose sole function is to be the Chief Laboratory Executive with authority to help determine and defend the research and development budget; to allocate the resources; to decide where work is being done; and to assess laboratory scientific, technical, and managerial performance."?

Answer: A "Laboratory Management Council" (LMC) has been created to coordinate policy management and overview of the laboratories. The council is comprised of senior executives of the Department who have responsibilities for or significant interests in the laboratories.

19. What is being done to implement the recommendation that "Consistent with the foregoing, modify the roles of the operations offices with respect to the laboratories to focus on management of the contracts with the laboratory operating contractors and to de-emphasize their function as policy and programmatic intermediaries between Headquarters and the laboratories."?

Answer: The Operations Office role in management of the laboratory contracts has been strengthened by the uniform laboratory appraisal process

recently implemented. Policy and programmatic guidance is focused within Headquarters.

20. **What is being done to implement the recommendation that DOE "Arrange for the laboratory directors to have substantially more flexibility, within overall budgets and broad program guidelines, to reprogram assigned laboratory resources and to initiate or adapt programs in accordance with research and development opportunities. This reprogramming authority should be no less than 5% or more than 10% subject to satisfactory completion of the original assigned program activity. If additional Congressional authorization for this reprogramming is needed, the Department should seek it."?**

Answer: The Congress has eliminated cost ceilings from its appropriation report language. Additional flexibility is supported by the DOE but will depend on Congressional action.

3.0 The Department's Policies and Procedures with Respect to the Laboratories

21. **What is being done to implement the recommendation that DOE "Utilize the services of an outside audit contractor familiar with both Government and industry practices to conduct a thorough audit of paperwork requirements in the Headquarters/operations offices/ laboratory chain of command."?**

Answer: The Assistant Secretary for Management and Administration has, in carrying out certain Management by Objectives initiatives, reported a reduction in Departmental paperwork by more than 30 percent. This includes the elimination of 32 reports, 923 forms, and 96,000 cubic feet of record and nonrecord material. A review of DOE directives by a committee of Deputy Assistant Secretaries identified a number of such documents for elimination or improvement. Thus far this fiscal year, 10 directives are being targeted for elimination and the reporting requirements are being reduced on 20 others. All reporting requirements have been identified and a program to review these in detail will be initiated shortly.

22. **What is being done to implement the recommendation that "To supplement internal appraisals of laboratory performance, the Department should convene panels from recognized scientific bodies, such as the National Academies of Science and Engineering, to conduct periodic (at intervals not greater than five years) technical audits of laboratory programs in connection with approved institutional plans."?**

Answer: To supplement internal appraisals, the Department has established an annual comprehensive appraisal process for the multiprogram laboratories. One of the key areas of review is quality of technical work. This review utilizes input from existing oversight panels such as the University of Chicago panel for Argonne National Laboratory. After some experience with the new appraisal process, the Department will evaluate its effectiveness and determine whether additional panels are required.

23. **What is being done to implement the recommendation that DOE "While maintaining priority status for essential Department missions, allow the laboratories to do more reimbursable work for others (other Federal agencies, state and local governments, and industry) be relaxing constraints on such work."?**

Answer: Consistent with the Atomic Energy Act, as amended, work-for-others policy and procedures are aimed at preventing laboratories from competing with industry; and insuring noninterference of mission work in making unique capabilities of the laboratories available to others. DOE has implemented an R&D Laboratory Technology Transfer Program responsive to the Stevenson-Wydler Act (P.L. 96-480). This program established DOE policy that since technology transfer activities at the laboratories have increased, the Department in consultation with the laboratories, has identified barriers to technology transfer and begun to resolve them. A series of "Spotlight on (name of laboratory)" in cooperation with the Industrial Research Institute (IRI) has been initiated to encourage industry access to facilities and to communicate work of potential commercial interest. Industry reaction has been quite favorable so far. To encourage R&D interactions, DOE has issued a class patent waiver for inventions arising from the reimbursable work-for-others. The response has been an increase in interactions with industry. The laboratories have established a close relationship with the IRI to stimulate interactions. The Secretary has assigned generic roles to the laboratories to provide for and encourage the transfer of technology.

24. **What is being done to implement the recommendation that DOE "Undertake a well-planned education program among Headquarters, operations office, and laboratory staff on the recently liberalized patent policy to ensure that it will be vigorously implemented. In parallel, ensure that the private sector understands the new policy."?**

Answer: Detailed documentation of the liberalized DOE patent waiver policy for work-for-others and laboratory user facilities has been circulated to all relevant departmental elements at Headquarters, in the field, and at the laboratories. Outreach to the private sector is an element of the R&D laboratory technology transfer program; the Office of Energy Research and Technology Assessment at each laboratory, as part of its job of facilitating interaction between the laboratory and industry, provides patent policy information. In January 1984, the "User's Guide to DOE Facilities" was completed and given wide distribution in university and industry sectors. The Guide is an important source of information for those interested in cooperative relationships among the national laboratories, the academic community and private industry.

4.0 Effectiveness of the Department's Use of the Laboratories in Meeting its Energy Objectives

25. **What is being done to implement the recommendation that DOE "Establish a consultant group of all laboratory directors to utilize more effectively laboratory resources in establishing the Department's research and development policy and directions."?**

Answer: Regular quarterly meetings are held with the directors of the multiprogram laboratories, the Director of Energy Research and program and administrative officials. Secretarial Offices attend as appropriate. A principal purpose of the meetings is to gain and utilize laboratory advice and resources in all important areas affecting the laboratories, including planning for research and development. In addition, each cognizant Secretarial official conducts an on-site review with the multiprogram laboratory

directors as part of the institutional planning process. Numerous meetings are also held at the program level including laboratory input to effective R&D program planning.

26. What is being done to implement the recommendation that DOE "implement vigorously the assignment of lead missions to the laboratories, defining these in terms of major applied programmatic missions, and provide for significantly greater laboratory discretion in allocation of resources (within overall Headquarters established budgets for the mission area) and in the selection of performers."?

Answer: The current Department lead mission concept has evolved into a specialized management tool which is used primarily to assign some significant authority and responsibility for technical program planning and direction to laboratories. Overall program planning and program budget direction remain with the Headquarters program office. A lead mission assignment cannot permit a laboratory to exercise any of the functions reserved exclusively to Government employees, by law. Lead mission assignments are encouraged for major efforts with a high technical content, involving reasonably stable, long-term assignments. They should be used only when authority and responsibility are not specifically established by contract or by organizational assignments.

27. What is being done to implement the recommendation that DOE "in setting research priorities, give special weight to making optimal productive use of sophisticated equipment and facilities."?

Answer: Program managers do place special emphasis on the use and scheduling of sophisticated equipment and facilities in the most efficient and effective manner possible. Increased utilization of energy intensive facilities is being sought by reducing power requirements through improvements in efficiency and requesting sufficient funds for adequate facility operation. DOE continues to seek the best possible rates for power through rate intervention and direct negotiation with utilities, as well as the use of off peak scheduling. In keeping with their overall roles and programs, the effort is to make these unique facilities available to members of the scientific and technical community, including both university and industry researchers.

28. What is being done to implement the recommendation that DOE "Establish user groups reporting to the Department, similar to the High Energy Physics Advisory Panel and the Nuclear Science Advisory Committee, for all of the Department's major mission programs and facilities. These could be established independently for each program function or under the umbrella of an overall advisory group."?

Answer: Several, but not all, programs would benefit from establishing such user groups. In addition to the High Energy Physics Advisory Panel (HEPAP) and the Nuclear Science Advisory Committee (NUSAC), the Department has established the Magnetic Fusion Advisory Committee (MFAC) and the Health and Environmental Research Advisory Committee (HERAC). MFAC has been in existence for over two years and HERAC was established just recently. The oversight panels for the Energy Reserch multiprogram laboratories have some user representation. Weapons laboratories have similar panels reporting to the University of California.

29. What is being done to implement the recommendation that DOE "Continue to support laboratory/university cooperation in the training of scientists and engineers through on-site participation by faculty and student in laboratory programs, term appointments, fellowships, etc."?

Answer: The laboratories contribute in the following ways:

1. Ensuring the availability of unique, user-oriented research facilities to university researchers (e.g., numerous facilities for High Energy Physics, and Basic Energy Sciences);

2. Providing research and training opportunities for a large number of undergraduate, graduate, and faculty researchers (e.g., up to 5,000 students have been assisted by the national laboratories through the use of laboratory facilities for their research, summer research appointments, etc.);

3. Subcontracting of research to university scientists;

4. Developing direct institution-to-institution links (most recently with a number of historically black colleges).

30. What is being done to implement the recommendation that DOE "Permit and encourage joint ventures in selected projects with industry, including test and pilot demonstration (located at the laboratories or on industrial sites) in order to test economic feasibility and to shorten the time lag for technology transfer."?

Answer: Present DOE policy permits joint R&D ventures with industry. The Department is addressing barriers which inhibit such ventures, such as patent rights. As far as pilot demonstrations and testing of economic feasibility is concerned, DOE generally considers these areas to be an industry, rather than a government responsibility.

31. What is being done to implement the recommendation that the DOE "In areas of special laboratory expertise and capabilities, allow and encourage the laboratories to work more closely with industry by such means as responding to requests for proposals from industry cooperative groups (e.g., American Society of Heating, Refrigeration, and Air-Conditioning Engineers; Electric Power Research Institute; and Gas Research Institute) and to work in partnership with industry in meeting technical needs of Federal agencies, as well as working directly for industry in connection with Federal agency requests for proposals."?

Answer: DOE laboratories, mainly government-owned and contractor operated, do not compete with the private sector by responding to requests for proposals. However, the laboratories are encouraged to be a useful resource to industry groups and make user facilities, reasonable consultation, and work-for-others support available.

32. What is being done to implement the recommendation that DOE "Permit each laboratory to use 1% to 2 % of its budget for independent research and development at the discretion of the laboratory director in order to enrich their research capabilities."?

Answer: On December 13, 1983, the Department issued a policy and guidelines for the use of a "reasonable amount of operating funds for early exploration and exploitation of creative and innovative scientific and technological concepts arising in the course of the laboratory's work."

33. What is being done to implement the recommendation that "Through a deliberative review and study by both the Department and the laboratories, identify institutional and doctrinal barriers to effective technology transfer and implement further action to ameliorate these."?

Answer: DOE requested and received input from laboratory directors on barriers to technology transfer as a prelude to a Headquarters meeting of senior laboratory personnel in 1983. A report documenting the recommendations of the meeting became the agenda for current Department efforts to improve the technology transfer program.

5.0 Alternative Strategies for Making Best Use of the Laboratories in a Constrained Budgetary Environment

34. What is being done to implement the recommendation that the DOE consider "Transferring appropriate DOE-sponsored work now performed by other Federal agencies and directing additional work into the laboratories by assigning to them those new tasks for which new laboratories might otherwise be established."?

Answer: There is relatively little DOE effort performed by other Federal Agencies. Work is given to other agencies when, and only when, the other agency can provide results in a more efficient, cost effective manner. The establishment of new laboratories is not contemplated and is not a current consideration.

35. What is being done to implement the recomendation that the DOE consider "Narrowing the missions of the laboratories to correspond to the resources available."?

Answer: The institutional planning process of the Department results in review of laboratory workload consistent with missions and quality of work. Determinations are made during the budget process to increase or decrease laboratory work depending on the availability of funds, and any overall change in missions or directions made as a result of Administration or Departmental policy. For example, mission redefinitions have resulted in some changes in laboratory size. The Laboratory Management Council, as part of its consideration of the 5-year institutional plans, reviews the proposed size of laboratories based on approved missions.

36. What is being done to implement the recommendation that the DOE consider "Closing particular laboratories or merging one or more of them with other DOE laboratories or even with other appropriate institutions outside the Department."?

Answer: There is no current activity or consideration being directed at the closing or merging of any of the Department's laboratories at this time.

D. White House Science Council Federal Laboratory Review Panel May 1983 Recommendations

1.0 Mission

37. What is being done to implement the recommendation that "As a top management priority, Federal agencies should reexamine the missions of their laboratories. Together with the laboratory directors, the agencies should redefine the missions as necessary to ensure that they are consistent with the appropriate roles for Federal laboratories. The missions must be made sufficiently clear and specific to guide the agency and the laboratories in setting goals against which the laboratories' performance can be evaluated."?

Answer: As part of the institutional planning process for FY 84-89, Secretary Hodel issued the Department's policy guidance for the role and missions of the multiprogram laboratories. The Secretary's policy guidance is based on his Congressional statement for the Federal role in energy R&D, and is consistent with the National Energy Policy Plan. The Laboratory Management Council (LMC) developed a general laboratory role statement, and reviewed and revised all proposed laboratory mission statements with special attention to their clarity and specificity. Beginning in 1984, annual laboratory appraisals will be carried out by the cognizant Operations Office to evaluate overall laboratory peformance in carrying out their missions.

38. What is being done to implement the recommendation that "The size of each Federal laboratory should be determined by the missions and the quality of its work. That size should be allowed to increase or decrease (to zero, if necessary) depending on mission requirements, but it should not fluctuate randomly. Preservation of the laboratory is not a mission."?

Answer: The institutional planning process of the Department results in review of laboratory workload consistent with missions and quality of work. Determinations are made during the budget process to increase or decrease laboratory work depending on availability of funds, and any overall change in missions or directions made as a result of Administration or Departmental policy. For example, mission redefinitions have resulted in some changes in laboratory size. The Laboratory Management Council, as part of its consideration of the 5-year institutional plans, reviews the proposed size of laboratories based on approved missions.

2.0 Resources: Personnel

39. What is being done to implement the recommendation that "Administrative and legislative actions should be initiated now to create, at government-operated, contractor-operated laboratories, a scientific/technical personnel system that is independent of current Civil Service personnel systems. The experimental system for managing scientific and technical personnel at the Naval Weapons Center and Naval Oceans Systems Center is an example of how this can be approached."?

Answer: The White House Science Council Federal Laboratory Review Panel Recommendation 2-1 pertains only to government-owned laboratories. Most of the Department's laboratories are government-owned, contractor-operated (GOCO) and their personnel systems are already independent of Civil Service, and of each other. The Federal Coordinating Council of Science, Engineering and Technology (FCCSET) has a Task Force chaired by the Department of the Navy that is preparing a recommendation regarding personnel systems for the government-operated laboratories.

40. What is being done to implement the recommendation that "Contracts governing government-owned, contractor-operated laboratories should be rewritten to permit the contractor to establish and carry out an independent salary administration."?

Answer: Government-owned, contractor-operated (GOCO's), under their current contracts with DOE, have the authority--in fact, the obligation--of setting up and administering their own salary and wage policies. DOE reviews and approves individual salary levels only of top laboratory management and senior research officials, and negotiates the overall rate of increase for personnel costs for each laboratory. The levels at which DOE review is required are adjusted periodically to reflect cost of living increases.

41. What is being done to implement the recommendation that "Personnel ceilings at government-operated laboratories should not be used in addition to budgetary control. Federal agencies should provide budget constraints and give the laboratory directors freedom to decide how to meet them. Laboratory directors should also be allowed to make the final decisions on contracting for support services at their laboratories."?

Answer: Headquarters works with the management of the DOE government-operated laboratories to establish the appropriate personnel complement within the limits established for the Department by OMB. All laboratory managements may decide on contracting for support services with broad policy guidelines based on the Department's and Federal acquisition regulations.

3.0 Resources: Funding

42. What is DOE doing to help implement the recommendation that "The Congress and Office of Management and Budget should authorize funding for R&D programs on a predictable multiyear basis so that staffing levels and research activities at Federal laboratories can be properly planned."?

Answer: The Secretary has supported this recommendation in meetings with laboratory directors, OSTP and Congress. DOE support was also noted in the Director of Energy Research's December 2, 1982 testimony.

43. What is being done to implement the recommendation that "At least 5 percent, and up to 10 percent, of the annual funding of the Federal laboratories should be devoted to programs of independent research and development at the laboratory directors' discretion. Federal agencies should establish a mechanism to evaluate the results of such work, with the size and continuation of discretionary funds related to laboratory performance. In order to encourage cooperative research programs, the laboratory directors should have

the authority, and be encouraged, to spend part of the discretionary funds at appropriate universities and industries."?

Answer: On December 13, 1983, the Department issued policy and guidelines for the use of a "reasonable amount of operating funds for early exploration and exploitation of creative and innovative scientific and technological concepts arising in the course of the laboratory's work." Managers of operations offices have the responsibility for monitoring and reporting on the use of such funding. Cooperative work with universities or private industry is not addressed. Encouragement of such cooperative efforts will be separated from the exploratory research and development authorized and encouraged by the new policy. Institutional planning will be the mechanism for evaluating overall results. The Laboratory Management Council will review the funding levels.

44. What is being done to implement the recommendation that "Federal laboratories should be allowed to carry forward remaining funds into the next fiscal year. This would eliminate the wasteful practice of hurried spending at the end of each fiscal year."?

Answer: Congress appropriates virtually all of the funds spent at DOE laboratories without fiscal year limitation. Consequently, unobligated balances routinely "carry over" into the succeeding fiscal years and remain available to the program. In the past Congressional committees have imposed cost controls; however, beginning with FY 1984 this ceiling limitation has been eliminated. For these reasons, there is no pressure for heavy end-of-year spending to prevent a lapse of funds. However, funds which are unobligated, while they do not lapse, are frequently applied by Congressional Appropriations Committees and OMB to finance part of the following year's program budgets. Therefore, there is a practical reason to obligate funds within the fiscal year to avoid the risk of having these funds picked up and used as budget offsets in the future.

Management

45. What is being done to implement the recommendation that "For each Federal laboratory, there should be an oversight function responsible for assuring the continuing excellence of the laboratory. This function could be performed by an external committee which should include strong industry and university representation. This committee would spend enough time at the laboratory to become familiar with the laboratory's strengths and weaknesses. It would focus on productivity and on excellence, relevance, and appropriateness of research. The oversight committee would make recommendations to the agency and inform the laboratory director of these recommendations. Those recommendations would be taken into account by the agency and laboratory in their budget decisions. In addition, the committee would give special attention to reducing micromanagement by the sponsoring agency."?

Answer: An oversight panel exists for Argonne National Laboratory (ANL) and Brookhaven National Laboratory (BNL), and is included in the new Oak Ridge National Laboratory (ORNL) contract. Weapons laboratories have similar

panels reporting to the University of California. DOE will examine existing external review mechanisms and whether they can be modified to meet the objectives of the recommendations. If not, additional mechanisms utilizing current committees, and possible new external committees, as recommended, will be evaluated.

46. **What is being done to implement the recommendation that "Federal agencies should rely to a greater extent on the competitive peer review process for funding basic research at their laboratories."?**

Answer: Several efforts have been made toward relying to a greater extent on peer review in funding specific Energy Research programs at the laboratories. In addition, a working group of affected program offices has been established to propose written guidance on how best to accomplish competitive peer review of basic research at laboratories. The Laboratory Management Council will review the proposed actions and recommend policy in this area.

47. **What is being done to implement the recommendation that "The laboratory director must be held accountable for the quality, relevance, and productivity of the laboratory. Appointment of the director should be for a finite term, with the option of extending or abbreviating the term depending on the performance of the director and the laboratory."?**

Answer: The concept of the management and operating contract (generally for a 5-year term), which DOE uses, has effectively enabled it to obtain the best managed R&D that the university and industry sectors can provide. The contractor chooses the person that can best direct the complex and diverse activities at a DOE-owned facility. The performance of each laboratory is appraised annually in the areas of overall management, program accomplishments, operations support, and administration. Implicit within the appraisal is the performance of the laboratory director. Near the end of the contract period when a determination is made as to whether or not to extend a contract, the performance of the laboratory director and the contractor are evaluated as part of the decision process.

48. **What is DOE doing to help implement the recommendation that "The above recommendations apply to all Federal agencies. The management of the Department of Energy presents an additional special problem, and the Panel recommends that the Administration and Congress work together to stabilize and strengthen DOE management and to define and reaffirm its mission. Congress should also refocus its oversight of DOE R&D into a significantly smaller number of committees."?**

Answer: Over the past seven years, the R&D part of DOE has evolved from the Atomic Energy Commission to the Energy Research and Development Administration and into the Department of Energy with concomitant change in mission and thrust of its R&D efforts. Over the last couple of years, there have been considerable efforts to sharpen the focus of these R&D efforts. Secretary Hodel, in a letter on July 28, 1983, issued the Department's policy guidance on the role and missions of the multiprogram laboratories. In October 1983, the National Energy Policy Plan IV was published and forwarded to Congress. Stabilization of funding in renewable energy, reductions in commercialization efforts, and an increased emphasis on the

appraisal of laboratory performance have, along with the foregoing, placed the Department in its best position to date to communicate and affirm its role and mission.

5.0 Interaction with Universities, Industry, and Users of Research Results

49. What is being done to implement the recommendation that "Federal laboratories should encourage much more access to their facilities by universities and industry."?

Answer: The implementation of the recommendation and encouragement to improve accessibility to laboratory facilities by university and industry has been included in the Department's Institutional Planning Process and the policy guidance to the laboratories. The "User's Guide to DOE Facilities" was completed in January 1984, and has been widely distributed to the university and industrial communities. The Guide will serve as an important source of information for those interested in cooperative relationships among the national laboratories, the academic community, and industry.

50. What is being done to implement the recommendation that "R&D interactions between Federal laboratories and industry should be greatly increased by more exchange of knowledge and personnel, collaborative projects, and industry funding of laboratory work, provided an oversight mechanism is established to prevent unfair competitive practices."?

Answer: The laboratories continue to be important complementary resources to university based research and education. Over 2000 university faculty members and students participate each year, generally during the summer, in laboratory-sponsored research and training programs. The budget for the DOE University Laboratory Cooperative Program has been significantly increased in FY 1985 to support additional faculty/student research appointments. Significant funding continues for the operation of major user-oriented research facilities at the laboratories, for example, about 40% of the Basic Energy Sciences budget in FY 1985 will support laboratory research facilities which are used by university scientists.

51. What is being done to implement the recommendation that "Contracting by agencies and laboratories for universities and industry to conduct R&D should be encouraged by simplifying the necessary Federal procurement procedures. The procurement process should give laboratory directors greater flexibility in contracting."?

Answer: Regarding university contracting procedures used by DOE, a working group has been established to recommend ways to simplify these procedures. As part of this process, DOE is converting many university awards from contracts to grants. Grants permit universities greater freedom in conducting their research. Also, emphasis has been placed on consistent interpretation of DOE university procurement regulations and procedures by all field elements. The Department will continue to review GOCO laboratory subcontracting activity as appropriate to ensure fairness and equity and general conformance to good practice.

40-574 O - 85 - 58

E. President's Private Sector Survey on Cost Control (PPSSCC)

52. Is this program responsible for implementing the recommendations of the PPSSCC study of the Department of Energy, and if not, who is responsible?

Answer: No, this program is not responsible for implementing the recommendations of the PPSSCC study. Those major recommendations of the PPSSCC study which will result in savings during FY 1984 and FY 1985 have been included in the DOE budget as Management Initiatives. DOE managers in all the Department's programs--both in Headquarters and in the field--are responsible for implementing the initiatives which are applicable to their program or organization. The Assistant Secretary for Management and Administration and her staff will monitor and coordinate this effort on a Department-wide basis.

53. What actions does DOE intend to take with regard to the PPSSCC study? What is the current status?

Answer: DOE has identified in the FY 1985 President's Budget to the Congress "management initiative savings" (which had their genesis in the PPSSCC as well as other review efforts) by program. These estimated savings of $47.5 million in FY 1984 and $96.0 million in FY 1985 are expected to be achieved as a result of implementation of a series of management initiatives. The initiatives involve improved management of deobligations, expanded audit efforts, improvements in DOE organization structure to reduce "layering" and improve our supervisor/employee ratios, increase reliance on the private sector for provision of commercial and industrial type support, reduction in procedural and reporting requirements to reduce Government and contractor overhead costs and other activities. Action on all of these initiatives is underway and at various stages of completion, oriented toward achieving savings in both FY 1984 and FY 1985. We also believe that implementation of these initiatives holds out the possibilities of additional savings in future years.

VI. MULTIPROGRAM GENERAL PURPOSE FACILITIES (MGPF)

1. **Please provide, for each of the multiprogram laboratories, the replacement value of existing general purpose facilities.**

Answer: Please refer to the table below.

Multiprogram General Purpose Facilities Program
Summary of Deficiencies and Replacement Value by Laboratory Sites
(In thousands of dollars)

Laboratory Sites	Requiring Rehabilitation	Requiring Replacement	Replacement Plant Value
Ames	$ 0	$ 3,350	$ 52,850
ANL	18,863	25,210	445,015
BNL	55,600	109,300	360,200
INEL	86,750	130,374	1,521,561
LANL	16,500	0	669,112
LBL	15,743	0	282,873
LLNL	16,600	40,420	254,890
ORNL	60,200	121,200	1,594,000
Richland	0	219,900	730,100
Sandia	47,000	100,000	860,000
Totals	$ 317,256	$ 749,754	$6,770,601

Source: Preliminary Institutional Plan for FY 1983-88.

2. **Please provide a summary of facility deficiencies and replacement value by DOE laboratory site.**

Answer: In the table below we list the total deficiencies and replacement plant value by each DOE laboratory site. The data are based on the 1982 Preliminary Institutional Plans.

Multiprogram General Purpose Facilities Program
(In thousands of dollars)

Laboratory Sites	Total Deficiencies	Replacement Plant Value
Ames	$ 6,700	$ 52,850
ANL	60,673	445,015
BNL	233,900	360,200
INEL	250,774	1,521,561
LANL	26,800	669,112
LBL	25,773	282,873
LLNL	119,730	254,890
ORNL	236,800	1,594,000
Richland	219,900	730,100
Sandia	261,000	860,000
Totals	$1,442,050	$6,770,601

The three kinds of deficiencies are (1) facilities requiring rehabilitation ($317 million), (2) facilities requiring replacement ($749 million), and (3) other needs ($375 million) to reduce overcrowding, improve reliability of

utilities and meet new environment, safety, and health requirements. The bulk of the deficiencies concern buildings ($996 million). Utility related deficiencies are estimated to be $324 million and all other deficiencies (e.g., roads, railways, etc.), $120 million.

The total list of deficiencies identified here includes all sized needs, both above and below $1 million dollars, and was prepared independent of the consideration of which program should fund them. Estimates for outyear projects are approximated by laboratory engineers.

3. **Provide a list, by site, of all the needed projects and the estimated cost of each.**

Answer: The projects listed below are those specifically identified by the laboratories in their Institutional Plans and/or Site Plans as being needed over the planning period FY 1986 - FY 1990. The total of all these projects is $460 million; this figure is somewhat less than the total backlog identified in Question 2. This lower amount reflects several factors. First, the total backlog of $1.4 billion dollars included all sized projects both above and below $1 million dollars as well as those that could be funded from landlord programs. Second, the $460 million reflects only well-defined line-items suitable for the MGPF program and a more realistic appraisal by the field of their needs vis-a-vis the observed funding activity of the MGPF program.

This project list is a snap-shot of what is expected to be required in future years. Because of changing R&D program directions, these lists may change as new deficiencies arise or existing ones get resolved via other means.

Project Title	B/A $ In Millions TEC
AMES MGPF	
Upgrade HVAC Metallurgical Building	1.0
Modifications to Former Reactor Building	1.1
TOTAL	2.1
ANL MGPF	
Water Line Replacement	6.0
Mechanical Systems Rehabilitation	3.0
Electric System Rehabilitation	5.1
Power House Rehabilitation	3.1
Transportation Facility	5.5
Central Supply Facility	10.5
TOTAL	33.2

Project Title	B/A $ In Millions TEC
BNL MGPF	
Fire Protection Improvements - Phase II	2.0
Applied Math Building Expansion	8.5
R&D Support Center	30.0
Boiler No. 1A Replacement	3.0
Central Shops Facility	11.5
TOTAL	55.0
LBL MGPF	
Electrical System Rehabilitation & Improvement	1.8
Engineering and Technical Support Facility	6.4
Building 50E 2nd Floor Addition	1.8
Building 50F 2nd Floor Addition	1.8
Corporation Yard, East Canyon Area	2.6
Rehabilitate or Replace Electronic Systems	3.8
Rehabilitate Site Mechanical Utilities	4.5
TOTAL	22.7
ORNL MGPF	
Upgrade Steam Distribution System	6.5
Utility Restoration - Piping System, Ph1 (Y-12)	4.0
Central Administration and Supply Building	5.5
Environmental Monitoring System Upgrade Ph2	5.0
Upgrade Fire Protection (Y-12)	1.9
Bioscience and Technology Facility	25.0
Utility Restoration - Electrical System, Ph1 (Y-12)	4.0
Electrical Distribution System Upgrade	1.5
Utility Restoration - Mechanical System, Ph1 (Y-12)	4.0
Existing Laboratories Upgrade	10.0
Technical Support Facility	15.0
Street System Rehabilitation & Additions	5.0
Support Facilities Upgrade	10.0
Existing Laboratory/Office Upgrade	13.0
Utility Restoration - Piping System, Ph2 (Y-12)	4.0
TOTAL	114.4

Project Title	B/A $ In Millions TEC
INEL MGPF	
Transportation Complex	9.4
Electrical & Telecommunications System Upgrade	4.9
Security Upgrade	10.0
Road Upgrade	3.5
Engineering Research Laboratory	22.0
INEL Security Buildings	2.8
INEL Road Upgrade	4.9
Multicraft Shop	1.5
INEL Electrical Upgrade-III	4.6
IER Laboratory	12.4
INEL Road Upgrade	5.0
INEL Electrical Upgrade-IV	5.0
Technical Office Building	11.9
INEL Road Upgrade	2.5
ILRC Computer Complex	6.4
ILRC Warehouse Facility	2.3
Electrical Upgrade-V	5.0
TOTAL	114.1
RL MGPF	
Multiprogram Support Technical Center, Ph1	5.0
Electrical Distribution System Upgrade, 300 Area Ph1	5.0
Steam Conditioning Return System Upgrade	3.0
Sewer System Upgrade, 300 Area	2.0
Fire, Radiation, Operations Safety Improvements, 300 Area	4.5
Energy Res. Laboratory Ph1, 300 Area	10.5
TOTAL	29.5
LANL MGPF	
Electronics Laboratory/Office Building	8.7
Pajarito Road Upgrade	2.0
Road Circulation Improvements	16.5
TOTAL	27.2
LLNL MGPF	
Earth Sciences Facility	13.9
Security & South Badge Office Facilities	6.3
Fire Facility	3.4
Motor Pool Facility	2.8
Site Entrance Improvements	4.0
Plant Engineering Shops Upgrade	7.2
Health & Safety Facility Additions	9.6
Supply & Distribution Facilities	8.5
Cafeteria/Auditorium Modification & Addition	1.7
TOTAL	57.4

Project Title	B/A $ In Millions TEC
SNL MGPF	
Information & Training Center	2.6
Document Storage Building	2.5
TOTAL	5.1

4. **In the FY 1984 budget request for MGPF, the Savannah River Laboratory (SRL) was included in the list of sites and facilities covered by the program. In the FY 1985 budget request for MGPF, SRL is no longer included. What is the reason for this change?**

   Answer: The facilities listed in the budget request are illustrative of those covered by the program. They are the ones most likely to receive program funds because of their multiprogram multipurpose nature. Savannah River Laboratory was not listed because it relies totally on a Defense Program funded upgrade program to fund needed projects. The MGPF program could cover a project there if it met the 60% test (i.e., no one program uses more than 60% of a proposed project).

5. **What criteria are used to determine whether or not a given project is to be funded by the (a) MGPF Program, (b) In-House Energy Management Program, and (c) General Plant Projects (GPP)?**

   Answer: The MGPF program funds only line-item sized projects (i.e. those above $1 million) that benefit two or more programs where no one program uses more than 60% of the facility involved. GPP funds can support any general plant projects with the Total Estimated Costs (TEC's) less than $1 million. The In-House Energy Management (IHEM) program funds both line-item and GPP sized projects; however, these projects must meet strict payback requirements based on energy cost savings. Payback is only one factor among many considered in the MGPF and GPP programs. Others include safety, health, environment, security, as well as programmatic need and impact.

   In general the MGPF program rehabilitates or replaces "multiprogram" facilities when they are deteriorated or constitute a hazard to personnel, operations or other facilities; whereas the IHEM program could replace a given facility if it meets their cost payback criteria (usually 3-5 years), GPP funding levels are established in Headquarters, but, the actual projects undertaken are determined in the field based on a process which determines the highest priority current need each has developed.

6. **What centralized management does DOE provide for the (a) MGPF Program, (b) In-House Energy Management Program, and (c) GPP?**

   Answer: All budgets are reviewed in terms of overall levels, issues and interactions at the Assistant Secretary level via the Internal Review Budget and the Institutional Planning processes. The MGPF and IHEM Programs operate agency-wide and their staffs coordinate their budget requests and activities continuously. The IHEM is managed by the Office of Project and Facilities Management, under the Assistant Secretary, Management and Administration. The MGPF Program is managed for the DOE by the Office of Field Operations Management under the Director, Office of Energy Research. The staff

a) provides overall program and budget review, b) delegates project execution responsibilities to the Operations Office and reviews performance periodically, c) does on-site reviews, and d) requests periodic reporting.

The GPP budget is also reviewed on both a Department-wide basis and also by each of the program offices responsible for managing specific GPP requirements. On a Department-wide basis GPP levels are reviewed by the Laboratory Management Council. At the program level the individual GPP project requests are reviewed on a more detailed basis both during the formulation and execution phase for each of the projects supported.

A. Hollfield Tables

7. The January 31, 1984 "Hollfield Tables" indicate that the IRB Fiscal Year 1985 budget request for the MGPF program totalled $60,000,000 for plant and capital equipment (PACE). According to these Tables, the Department's FY 1985 submission to OMB for the program totalled $44,750,000 for PACE. What are the specific differences between these two budgets?

Answer: The following table reflects the projects that were changed from the IRB Request to the OMB submission:

		($ In Thousands)		
		FY 1985	FY 1985	
Project#	Title	IRB Request	OMB Request	Change
	On-going projects.....	$ 21,942	$ 21,942	$ 0
85-R-700	Facility Support, various locations.....	4,991	0	- 4,991
85-R-701	Central Chilled Water Facility, BNL.....	3,500	3,500	0
85-R-702	Replace Laboratory Roofs, ANL.....	4,800	3,300	- 1,500
85-R-703	Primary Electrical Distribution System, ORNL.....	2,200	1,100	- 1,100
85-R 704	Rehabilitate Underground Steam System, ANL.....	1,767	3,000	+ 1,233
85-R-705	Electric & Telecommunication System, INEL.....	2,400	708	- 1,692
85-R-706	Medical Facility, LLNL...	2,500	3,400	+ 900
85-R-707	Hanford Site Fire Alarm System Upgrade, HEDL....	2,800	1,300	- 1,500
85-R-708	Facility Support, various locations.....	6,400	0	- 6,400
85-R-709	Central Chilled Water Plant, ANL.....	2,500	1,000	- 1,500
85-R-710	Utilities Restoration Piping System, ORNL.....	1,500	1,500	0
85-R-711	Upgrade Environmental Monitoring, ORNL.....	1,000	1,000	0
85-R-712	Central Chilled Water System Restoration, ORNL	1,700	1,000	- 700
85-R-713	Replace Transportation Complex, INEL.....	0	2,000	+2,000
	Total MGPF.....	$ 60,000	$ 44,750	$-15,250

8. **As noted in question 1 above, the Holifield Tables indicated that the OMB FY 1985 budget request for the MGPF totalled $44,750,000 for PACE. The FY 1985 Congressional request for MGPF totalled $38,950,000 for PACE. What are the specific differences between these two budgets?**

Answer: The following table reflects the projects that were changed from the OMB Request to the Congressional submission:

Project#	Title	FY 1985 IRB Request ($ In Thousands)	FY 1985 OMB Request ($ In Thousands)	Change ($ In Thousands)
	On-going projects.....	$ 21,942	$ 21,942	$ 0
85-R-701	Central Chilled Water Facility, BNL.....	3,500	3,500	0
85-R-702	Replace Laboratory Roofs, ANL.....	3,300	3,508	+ 208
85-R-703	Primary Electrical Distribution System, ORNL.....	1,100	1,100	0
85-R 704	Rehabilitate Underground Steam System, ANL.....	3,000	3,000	0
85-R-705	Electric & Telecommunication System, INEL.....	708	0	- 708
85-R-706	Medical Facility, LLNL...	3,400	1,600	- 1,800
85-R-707	Hanford Site Fire Alarm System Upgrade, HEDL....	1,300	1,300	0
85-R-709	Central Chilled Water Plant, ANL.....	1,000	1,000	0
85-R-710	Utilities Restoration Piping System, ORNL.....	1,500	0	- 1,500
85-R-711	Upgrade Environmental Monitoring, ORNL.....	1,000	1,000	0
85-R-712	Central Chilled Water System Restoration, ORNL	1,000	1,000	0
85-R-713	Replace Transportation Complex, INEL.....	2,000	0	-2,000
	Total MGPF.....	$ 44,750	$ 38,950	$- 5,800

9. **Given the information in questions 7 and 8 above, what are the specific differences between the FY 1985 IRB and the Congressional Request budgets for MGPF?**

Answer: The following table reflects the projects that were changed from the IRB Request to the Congressional submission:

Project#	Title	FY 1985 IRB Request	FY 1985 OMB Request	Change
		($ In Thousands)		
	On-going projects.....	$ 21,942	$ 21,942	$ 0
85-R-700	Facility Support, various locations.....	4,991	0	- 4,991
85-R-701	Central Chilled Water Facility, BNL.....	3,500	3,500	0
85-R-702	Replace Laboratory Roofs, ANL.....	4,800	3,508	- 1,292
85-R-703	Primary Electrical Distribution System, ORNL.....	2,200	1,100	- 1,100
85-R 704	Rehabilitate Underground Steam System, ANL.....	1,767	3,000	+ 1,233
85-R-705	Electric & Telecommunication System, INEL.....	2,400	0	- 2,400
85-R-706	Medical Facility, LLNL...	2,500	1,600	- 900
85-R-707	Hanford Site Fire Alarm System Upgrade, HEDL....	2,800	1,300	- 1,500
85-R-708	Facility Support, various locations.....	6,400	0	- 6,400
85-R-709	Central Chilled Water Plant, ANL.....	2,500	1,000	- 1,500
85-R-710	Utilities Restoration Piping System, ORNL.....	1,500	0	- 1,500
85-R-711	Upgrade Environmental Monitoring, ORNL.....	1,000	1,000	0
85-R-712	Central Chilled Water System Restoration, ORNL	1,700	1,000	- 700
	Total MGPF.....	$ 60,000	$ 38,950	$-21,050

B. Projects

1.0 Project 85-R-701, Central Chilled Water Facility (BNL)

10. Is this project's September 1983 cost estimate of $15,000,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $15,000,000 is in as-year spent dollars.

11. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: This estimate was escalated to the midpoint of construction using the following escalation rates: FY 1983 - 9.6%, FY 1984 - 9.0%, FY 1985 - 8.9%, FY 1986 - 8.5%, and FY 1987 - 8.5%. These are the rates issued by DOE ("FY 1982 Guidance, Anticipated Economic Escalation Rates for DOE Construction Projects"). Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will

start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place. In this particular case the midpoint of construction is in FY 1987.

12. Reoptimize the project's funding profile for a one-year slippage in the construction end date (i.e., from 3rd Qtr. FY 1988 to 3rd Qtr. FY 1989). How much would this escalate the project's cost? What assumptions are used to estimate this escalation?

Answer: The current funding profile is FY 1985 - $3,500,000, FY 1986 - $7,500,000, FY 1987 - $4,000,000. The reoptimized funding profile for a one-year slippage in the construction end date is FY 1985 - $1,500,000, FY 1986 - $6,500,000, FY 1987 - $4,000,000, FY 1988 - $34,00,000. A slippage of one year based on the above escalation rates would add approximately $400,000 to project costs. A one-year slippage in the construction end date means a 1/2-year slippage in the midpoint of construction. Therefore, the estimated cost of construction is increased by 1/2 of the projected escalation in FY 1987 (1/2 of 8.5%).

2.0 Project 85-R-702, Replace Laboratory Roofs (ANL)

13. Is this project's December 1983 cost estimate of $9,800,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The December 1983 cost estimate of $9,800,000 is in as-year spent dollars.

14. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: This estimate was escalated to the midpoint of construction using the following escalation rates: FY 1984 - 5.4%, FY 1985 - 6.8%, FY 1986 - 7.2%, FY 1987 - 7.0%, FY 1988 - 7.1%, and FY 1989 - 7.2%. These are rates issued by DOE ("2nd Quarter CY 1983 Update to FY 1983 Guidance, Anticipated Economic Escalation Rates for DOE Construction Projects"). Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

3.0 Project 85-R-703, Electrical Distribution System Rest. (ORNL)

15. Is this project's September 1983 cost estimate of $2,200,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $2,200,000 is in as-year spent dollars.

16. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: This estimate was escalated to the midpoint of construction using the following escalation: FY 1983 - 8.0%, FY 1984 - 8.5%, FY 1985 - 8.5%, FY 1986 - 8.5%, and FY 1987 - 8.5%. These escalation rates were based on annual escalation studies conducted by the Oak Ridge Operations Office in areas of building, equipment and materials, and labor costs. The mix of these costs is determined for each project and accordingly the escalation rate is calculated. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

4.0 Project 85-R-704, Rehab. Underground Steam System (ANL)

17. Is this project's September 1983 cost estimate of $3,000,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $3,000,000 is in as-year spent dollars.

18. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: The estimate was escalated to the midpoint of construction using the following rates: FY 1984 - 5.4%, FY 1985 - 6.8%, FY 1986 - 7.2%, FY 1987 - 7.0%, FY 1988 - 7.1%, and FY 1989 - 7.2%. The escalation rates were issued by DOE (2nd Quarter Update to FY 1983 rates). Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

5.0 Project 85-R-706, Medical Facility Replacement (LLNL)

19. Please provide a construction project data sheet for this project.

Answer: Please find a construction project data sheet attached.

DEPARTMENT OF ENERGY
FY 1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Medical Facility
Lawrence Livermore National Laboratory
Livermore, California

2. Project No.: 85-R-706

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 1st Qtr. FY 1986

4. Date Construction ends: 1st Qtr. FY 1988

5. Previous cost Estimate: None
Date: none

6. Current cost estimate: $ 7,300
Less amount for CP&D: 0
Net cost estimate: $ 7,300

Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 7,300	$ 1,600	$ 1,600	$ 300
1986	0	4,800	4,800	4,000
1987	0	900	900	3,000

8. Brief Physical Description of Project

This project will provide a 25,600 gross square foot building for a new and expanded facility for Health Services and will house all of the 32 medical staff and support personnel. The functions accommodated in this space will be a waiting area, receptionist, interview rooms, administrative offices, records area, health maintenance offices, physical examination rooms, observation room, emergency treatment (major and minor), diagnostic laboratories, specimen rooms, X-ray room, dark room/process lab, autoclave and clean hold area, ambulance entry, personnel decontamination facility, eye safety examination rooms, toilets, storage and equipment rooms.

The building will be designed to relate to the existing nearby major facilities and will be constructed of fire-resistive materials. Fire sprinkler system as well as other safety devices, will be installed. Normal medical laboratory building utilities, heating, ventilation, power, lighting, and communication systems will be provided. The building will be cooled by mechanical refrigeration. In addition, the decontamination area will require special ventilation, sewage retention tanks, and floor treatment. Energy conserving design will be utilized throughout the facility.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Medical Facility
Lawrence Livermore National Laboratory
Livermore, California

2. Project No.: 85-N-706

8. Brief Physical Description of Project (continued)

Normal site utilities will be extended from mains and connections to storm and sanitary sewers will be made. Electrical power will be extended from high voltage feeders to a new substation serving this building. Area lighting will be installed for safety and security. Site development will comply with the Master Site Plan and will include grading, paving, off-street parking, curbs, gutters, sidewalks, fencing, security screens, and minimal landscaping.

9. Purpose, Justification of Need for, and Scope of Project

Adequate health service support to the over 7600 employees of LLNL primarily consists of two major elements. First, preventative approaches to both the physical and mental health of the workforce. This is accomplished through performance of over 3500 physical examinations a year, attention to the potential hazards of one of the country's foremost applied physics and engineering facilities and support to those who may be unduly stressed by working in such an environment. Second, is the availability of adequate emergency response to a very broad spectrum of hazards ranging from intense radioactivity, through almost every possible chemical, mechanical and electrical risk, to the "normal" falls, cuts, etc., that go with a dynamic population that includes over a thousand contractor employees in addition to the LLNL staff. Although blessed with one of the best safety records of the national laboratories, the health services facility must be prepared for major incidents.

The current health facility is housed in a 40 year old World War II barracks building that is shared with the South Badge Office. It was barely adequate for a medical staff of less than 20 and a population of less than 5000. Today the building limits physical examinations to approximately two thirds of the DOE guidelines for a laboratory of LLNL's size. Several other health services required by DOE order, DOT regulation, California code, ANSI standards, and LLNL policy are currently not being provided due to the physical restraints of the current building. For example, in the event of persons being contaminated with radioactive, toxic, or carcinogenic materials, they cannot be adequately treated without significant risk to the current facility and attending personnel. A special unit needs to be constructed to deal with this particular type of emergency situation. The present facility is generally not capable of handling a large variety of emergency situations nor a large number of casualties.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Medical facility
Lawrence Livermore National Laboratory
Livermore, California

2. Project No.: 85-R-706

10. Details of Cost Estimate*

	Item Cost	Total Cost
a. Engineering, design, and inspection at approximately 13% of construction costs		
1) Title I & II	$ 400	
2) Title III	300	
		$ 700
b. Construction costs		5,550
1) Improvements to Land including grading, paving, walks and landscaping	550	
2) Buildings		
Medical, 25,600 sq. ft. at $162 per sq. ft.	4,150	
3) Utilities, including mechanical, power, communications, storm and sanitary sewer	850	
c. Standard equipment		140
d. Relocation cost		100
Subtotal		$ 6,490
f. Contingency at approximately 12% of other costs (except item a. and c. above)		810
Total Project Cost		$ 7,300

*Based on complete conceptual design.

11. Method of Performance

This project will be designed and constructed under a procedure commonly referred to as turnkey contracting. The project will be competitively bid with each bidder submitting a design and cost proposal. Minor work will be performed by LLNL forces.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Medical facility
Lawrence Livermore National Laboratory
Livermore, California

2. Project No.: 85-R-706

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1985	FY 1986	FY 1987	Total
a. Total Project Funding					
1. Total Facility Costs					
a. Construction line item	$ 0	$ 300	$ 4,000	$ 3,000	$ 7,300
b. CP&D	0	0	0	0	0
c. Expense funded equipment ..	0	0	0	0	0
d. Inventories	0	0	0	0	0
Total direct costs	$ 0	$ 300	$ 4,000	$ 3,000	$ 7,300
2. Other Project Funding					
a. R&D necessary to complete construction	120	0	0	0	120
b. Other project related costs	0	0	0	0	0
Total other project costs	120	0	0	0	120
Total project costs	$ 120	$ 300	$ 4,000	$ 3,000	$ 7,420

b. Other related annual costs (Estimated Life of Facility: 40 years)	
1. Facility operating costs	$ 230
2. Programmatic operating expenses directly related to the facility	3,280
3. Capital equipment not related to construction but related to the programmatic effort in the facility	300
4. GPP or other construction related to programmatic effort in the facility	100
5. Other costs	0
Total other related annual funding costs	$ 3,910

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project:	Medical facility Lawrence Livermore National Laboratory Livermore, California	2. Project No.: 85-R-706

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding

1. Total facility costs
   a. Construction line item - No narrative required.
   b. Expense funded equipment - No narrative required.
   c. Inventories - No narrative required.
2. Other project funding
   a. R&D necessary to complete construction
      Total funding in this classification represents the conceptual design cost and other studies determined to be necessary.
   b. Other related project cost - No narrative required.

b. Total related-funding requirements

1. Facility operating costs
   Operating costs of the facility are estimated to be $226,000 per year including $92,900 escalation (based on FY 1982 average maintenance and utility cost of $5.20 per sq. ft. escalated to $8.83 in FY 1987. Maintenance cost escalated at 7% per annum, and utility cost escalated at 15% per annum).

2. Programmatic operating expenses directly related to the facility
   This estimate is for 32 total programmatic and support personnel at $102,540 average per person in FY 1987. Ninety percent of these people are presently housed in existing scattered buildings and trailers and will be moved to this new facility. The operating funds for these people are a normal part of the past and current programs. The remaining 10 percent represent growth projected to FY 1987. Funds for this growth have been included in program projections.

3. Capital equipment not related to construction but related to the programmatic effort in the facility
   This is an average annual estimate which includes both the small items needed for continuous operation of the facility and the occasional large item over $100,000 which cannot be described at this time, but can be predicted as needed to maintain technical excellence in efforts conducted in the facility.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Medical Facility
Lawrence Livermore National Laboratory
Livermore, California

2. Project No.: 85-R-706

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements (continued)

4. GPP or other construction related to programmatic effort
Initially no GPP costs are anticipated but to keep abreast of technology, presently undefined alterations will likely be required in the future.

5. Other costs - No narrative required.

20. Is this project's cost estimate of $7,300,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The project's cost estimate of $7,300,000 is in as-year spent dollars.

21. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: This estimate was escalated to the midpoint of construction using the following rates: FY 1983 - 5.6%, FY 1984 - 7.0%, and 8.0% for each year thereafter. These escalation rates were based on LLNL surveys of nationally known professional cost estimators' projections and statistically averaged to provide normalized results for the LLNL area. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

6.0 Project 85-R-707, Replace Site Fire Alarm System (RL)

22. Is this project's September 1983 cost estimate of $4,850,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $4,850,000 is in as-year spent dollars.

23. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates use?

Answer: This estimate was escalated to the midpoint of construction using the following rates: FY 1984 - 7.2%, FY 1985 - 7.9%, and FY 1986, 8.2%. These escalation rates were based on studies conducted by the Richland Operations Office for the Washington area. The study utilized the escalation model developed by Data Resources, Inc. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

7.0 Project 85-R-709, Est. Central Chilled Water Plant (ANL)

24. Is this project's September 1983 cost estimates of $5,200,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $5,200,000 is in as-year spent dollars.

25. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: The estimate was escalated to the midpoint of construction using the following rates: FY 1984 - 5.4%, FY 1985 - 6.8%, FY 1986 - 7.2%, FY 1987 - 7.0%, FY 1988 - 7.1%, and FY 1989 - 7.2%. These rates were issued by DOE (2nd Quarter CY 1983 Update to FY 1983 rates). Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

8.0 Project 85-R-711, Upgrade Environmental Monitoring (ORNL)

26. Is this project's September 1983 cost estimate of $3,500,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $3,500,000 is in as-year spent dollars.

27. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: The estimate was escalated to the midpoint of construction using the following rates: FY 1984 - 5.5%, FY 1985 - 7.0%, FY 1986 - 7.0%, FY 1987 - 7.0%, and FY 1988 - 7.0%. These escalation rates were based on annual studies conducted by the Oak Ridge Operations Office on the areas of building, equipment and materials, and labor costs. The mix of these costs are determined for each project and accordingly the escalation rate is calculated. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

9.0 Project 85-R-712, Modify Central Chilled Water Plant (ORNL)

28. Is this project's September 1983 cost estimate of $4,700,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The September 1983 cost estimate of $4,700,000 is in as-year spent dollars.

29. What escalation rate estimates are used over the life of the project? What was the basis for the escalation estimates used?

Answer: This estimate was escalated to the midpoint of construction using the following rates: FY 1984 - 5.5%, FY 1985 - 7.0%, FY 1986 - 7.0%, and FY 1987 - 7.0%. These escalation rates were based on annual studies conducted by the Oak Ridge Operations Office in the areas of building, equipment and

materials, and labor costs. The mix of these costs are determined for each project and accordingly the escalation rate is calculated. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

10.0 Project 84-ER-103, Road Repair (LBL, INEL, RL, ANL)

30. **Is this project's August 1982 cost estimate of $16,000,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?**

Answer: The August 1982 cost estimate of $16,000,000 is in as-year spent dollars.

31. **What escalation rates were assumed in the August 1982 estimate? How have the actual escalation rates compared with the August 1982 estimates?**

Answer: The estimates of the individual subprojects were escalated to the midpoint of construction using the following rates:

LBL* - FY 1983 - 8.0%, FY 1984 - 8.5%, and FY 1985 - 9.0%

INEL - FY 1982 - 10.7%, FY 1983 - 11.6%, FY 1984 - 11.6%, and FY 1985 - 11.6%

RL - FY 1982 - 9.4%, FY 1983 - 9.8%, FY 1984 - 9.0%, and FY 1985 - 8.8%

ANL* - FY 1984 - 5.8%, FY 1985 - 7.8%, and FY 1986 - 8.1%

*Projects were reestimated in 1983.

Actual escalation rates were:

LBL - FY 1983 - 4.7%

INEL - FY 1983 - 4.7%

RL - FY 1983 - 2.0%

ANL - FY 1983 - 3.4%

Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

32. **What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the August 1982 estimate?**

Answer: The overage due to the difference in estimated and actual escalation rates is $1,146,000. The August 1982 estimate has not changed because actual escalation rates for FY 1984 and beyond are not known at this time.

33. **How much of the project's total contingency of $1,975,000 remains? How much of the $630,000 contingency at Richland remains? How much of the $955,000 contingency at INEL remains? How much of the $190,000 contingency at LBL remains? How much of the $200,000 contingency at ANL remains?**

Answer:

Richland - The design is approximately 30% complete and the A-E has not yet completed a construction estimate. The present working estimate for design is $390,000 compared with the 1982 estimate of $295,000. This leaves $535,000 contingency remaining.

INEL - Since design is still underway (10% complete) and the project has not been bid yet, it is difficult to determine the present status of the contingency funds. Until further definitization the $955,000 contingency remains.

LBL - Since authorization, as a result of the negotiated fee for the A-E and reworking of estimated costs for outside consultants (soils engineer, surveyor, testing laboratory, etc., the remaining contingency is $100,000 which is approximately 9.4% of the construction cost.

ANL - All of the $200,000 contingency remains due to the fact that this project is currently in the early Title I design stage. Construction is not scheduled to start until July 1984.

34. **Why are there site-to-site variances in the ratios of the engineering and design and inspection (EDI) estimates to the construction cost estimates for this project? For example, this ratio is 0.138 for Richland, 0.088 for INEL, 0.158 for LBL, and 0.125 for ANL. What are the reasons for these variances?**

Answer: EDI costs are dependent on several variables: (1) scope of work: The scope of work varies from project to project at these laboratories. LBL has a considerable amount of earthwork involved in its road repair; consequently there is considerable more field work required (surveying and design). On the other hand much of the work at INEL involves only the addition of a leveling course of asphalt (minimum surveying and design). The work at RL and ANL include the removal, relocation, and repair of more utilities than at INEL. Generally as the TEC of road projects increases the percentage of EDI decreases. (2) Method of Accomplishment: LBL and RL plan to accomplish the design and inspection by a negotiated architect-engineering contract while INEL and ANL plan to use laboratory personnel for design and inspection. Because laboratory personnel are more familiar with the site and scope of work they will be able to accomplish the work at less cost than an A-E. (3) Location: A-E firms in the San Francisco Bay Area on the average charge more than A-E firms in Richland for comparable work.

35. **Why are there site-to-site variances in the ratios of the contingency estimates to the construction plus EDI cost estimates for this project? For example, these ratios are 0.144 for Richland and INEL, 0.157 for LBL, and 0.111 for ANL. What are the reasons for these variances?**

Answer: The amount of contingency depends on the complexity and uncertainties of each project's component parts. For example, the contingency at LBL was higher than the others because the site is located on a hillside and the geological conditions are complex; consequently subsurface conditions are variable and less predictable than the conditions that are found on flat sites. ANL contingency is lower than the others because of ANL project management's knowledge of existing conditions for this particular project. Also taken into consideration by ANL was the historical experience of construction project costs. Contingency is determined by each site based on an analysis of each project's complexity and uncertainties.

11.0 Project 84-ER-102, Cooling Water Facility Rest. (ORNL)

36. **Is this project's April 1982 cost estimate of $4,000,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?**

Answer: The April 1982 cost estimate of $4,000,000 is in as spent dollars.

37. **What escalation rates were assumed in the April 1982 estimate? How have the actual escalation rates compared with the April 1982 estimate?**

Answer: The estimate was escalated to the midpoint of construction using the following rates: FY 1983 - 8.0%, FY 1984 - 8.5%, FY 1985 - 8.5%, FY 1986 - 8.5%, and FY 1987 - 8.5%. Actual escalation rate for FY 1983 was 3.0%. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

38. **What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the April 1982 estimate?**

Answer: The overage that has occurred because of the difference in the estimated and actual escalations rates is $24,000. The April 1982 estimate has not changed because actual escalation for FY 1984 and beyond is not known at this time.

39. **How much of the project's $475,000 contingency remains?**

Answer: All of the project's $475,000 contingency remains at the 30% completion phase.

12.0 Project 84-ER-101, Rehab. Old Town Utilities (LBL)

40. Is this project's March 1982 cost estimate of $4,750,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The March 1982 cost estimate of $4,750,000 is in as-year spent dollars.

41. What escalation rates were assumed in the March 1982 estimate? How have the actual escalation rates compared with the March 1982 estimates?

Answer: The estimate was escalated to the midpoint of construction using the following rates: FY 1982 - 11.0%, FY 1983 - 9.3%, FY 1984 - 9.1%, and FY 1985 - 8.4%. Actual escalation rates for the San Francisco area based on Engineering News Record Building Index were: 1981 - 8.3%, 1982 - 9.4%, and FY 1983 - 4.7%. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

42. What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the March 1982 estimate?

Answer: The overage that has occurred because of this difference is $210,000. The March 1982 estimate has not changed because actual escalation is not known for FY 1984 and beyond.

43. How much of the project's $430,000 contingency remains?

Answer: The current estimated cost of the major construction components of the project remain unchanged, however, the A-E fee negotiated for the project is $80,000 higher than originally estimated. No change in TEC is anticipated. However, the contingency has been reduced to $350,000 to accomodate the higher A-E fee.

13.0 Project 83-E-310, Utility Replacement and Upgrade (BNL)

44. Is this project's June 1981 cost estimate of $12,000,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The June 1981 cost estimate of $12,000,000 is in as-year spent dollars.

45. What escalation rates were assumed in the June 1981 estimate? How have the actual escalation rates compared with the June 1981 estimate?

Answer: This estimate was escalated to the midpoint of construction using the following rates: FY 1982 - 10%, FY 1983 - 10%, and FY 1984 - 10%. The actual escalation rates per Data Resources, Inc. were: FY 1981 - 7.9%, FY 1982 - 6.6%, and FY 1983 - 6.8%. Generally the cost estimate is completed

two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

46. What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the June 1981 estimate?

Answer: The overage due to escalation differences is $440,000 at this time. The June 1981 estimate has not changed because (1) the actual escalation for FY 1984 and FY 1985 are not known at this time and (2) the project has been delayed approximately six months because of the continuing resolution.

47. How much of the project's $1,600,000 contingency remains?

Answer: At present $1,600,000 remains. This is based on design not being complete at this time.

14.0 Project 83-E-309, Electronics Facility (ANL)

48. Is this project's January 1981 cost estimate of $8,500,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The January 1981 cost estimate of $8,500,000 is in as-year spent dollars.

49. What escalation rates were assumed in the January 1981 estimate? How have the actual escalation rates compared with the January 1981 estimate?

Answer: This estimate has been escalated to the midpoint of construction using the following rates: 10% per year. Actual escalation rates based on Means Construction Cost Indices since January 1981 have been: 1981 - 9.4%, 1982 - 5.3%, and 1983 - 3.4%. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

50. What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the January 1981 estimate?

Answer: The overage due to escalation differences is $1,275,000 at this time. The January estimate has not changed because actual escalation in FY 1984 and beyond are not known at this time.

51. How much of the project's $1,130,000 contingency remains?

Answer: With Title II at 75% completion and approximately 10% of construction in place or negotiated, remaining contingency is $840,000. This represents 11.8% of the total of $7,100,000 not costed or committed to date.

15.0 Project 83-E-308, Rehab. Power Systems (INEL, LLNL, RL, ORNL)

52. Is this project's April 1981 cost estimate of $15,830,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The April 1981 cost estimate of $15,830,000 is in as-year spent dollars.

53. What escalation rates were assumed in the April 1981 estimate? How have the actual escalation rates compared with the April 1981 estimates?

Answer: The estimates of the individual subprojects were escalated to the midpoint of construction using the following rates:

INEL: FY 1981 - 10.7%, FY 1982 - 11.8%, FY 1983 - 11.6%, and FY 1984 - 11.6%

LLNL: 12% for each year FY 1981 - FY 1984

RL: FY 1981 - 12%, and 11% for each subsequent year

ORNL: 10% for each year FY 1981 - FY 1985

Actual Escalation Rates:

INEL: FY 1981 - 12.5%, FY 1982 - 6.4%, and FY 1987 - 4.7%

LLNL: FY 1981 - 9.3%, FY 1982 - 6.9%, and FY 1983 - 5.5%

RL: FY 1981 - 11.7%, FY 1982 - 7.0%, and FY 1983 - 2.0%

ORNL: FY 1981 - 9.8%, FY 1982 - 3.5%, and FY 1983 - 3.0%

Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

54. What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the April 1981 estimate?

Answer: The overage due to the difference in the estimated and actual escalation rates is $821,000. The April 1981 estimate has not changed because the actual escalation in FY 1984 and beyond is not known at this time.

55. How much of the project's total contingency of $2,140,000 remains? How much of the $660,000 contingency at INEL remains? How much of the $180,000 contingency at LLNL remains? How much of the $600,000 contingency at Richland remains? How much of the $700,000 contingency at ORNL remains?

Answer:

INEL - Due to the fact that design is only 20% complete, it is difficult to determine the actual amount of remaining contingency. Until further definitization of design is complete, it is assumed the full $660,000 remains.

LLNL - Currently all of the $180,000 contingency remains. However, design has just recently been completed and bids have not yet been received for construction. Lab personnel are currently evaluating transformer bids that range from $450K to $890K.

RL - $408,000 contingency remains.

ORNL - Currently all of the $700,000 contingency remains.

56. **Why are there site-to-site variances in the ratios of the engineering and design and inspection (EDI) estimates to the construction cost estimates for this project? For example, this ratio is 0.0625 for Richland, 0.122 for INEL, 0.148 for LLNL, and 0.162 for ORNL. What are the reasons for these variances?**

Answer: EDI costs are dependent on (1) scope of work (2) method of accomplishment and (3) variance in A-E fees. While these four subprojects fall into the category of rehabilitation of power systems they have different scopes of work with varying degrees of complexity. For example, the INEL, LLNL and ORNL projects include some high voltage (greater than 115,000 volts) work, while the Richland scope of work includes distribution voltage (13,800 volts) only. While the data sheet shows the EDI work at Richland being accomplished by a negotiated contract with an A-E firm, the estimate was based on the work being accomplished in-house. In-house costs are usually less than negotiated contracts with an A-E firm because of the familiarity with the project. Another reason for variance is the price charged by local A-E firms. The A-E rates vary from site-to-site.

57. **Why are there site-to-site variances in the ratios of the contingency estimates to the construction plus EDI cost estimates for this project? For example, these ratios are 0.176 for Richland, 0.156 for INEL, 0.103 for LLNL, and 0.163 for ORNL. What are the reasons for these variances?**

Answer: The amount of contingency depends on the complexity and uncertainties of each subproject's component parts. With each subproject having a different scope of work the uncertainties will be different. For example, the work at Richland includes more than 1/2 mile of underground work. With the probability that there are uncharted utilities within the excavation area the uncertainty risks increases. LLNL on the other hand determined that less than 15% contingency would be adequate based on only minor underground (less than 100 feet) work and use of construction techniques that are well established. Contingency is determined by each site based on an analysis of each project's complexity and uncertainties.

16.0 Project 82-E-302, Security Facility (ANL)

58. Is this project's May 1980 cost estimate of $8,100,000 in FY 1984 dollars, FY 1985 dollars, or in as-year spent dollars?

Answer: The May 1980 cost estimate of $8,100,000 is in as-year spent dollars.

59. What escalation rates were assumed in the May 1980 estimate? How have the actual escalation rates compared with the May 1980 estimate?

Answer: This estimate was escalated to the midpoint of construction using the following rates: FY 1980 - 12%, FY 1981 - 12%, FY 1982 - 11%, FY 1983 - 10%, FY 1984 - 10%, and FY 1985 - 10%. Actual escalation based on Means Construction Cost Indices during this period were: FY 1980 - 9.3%, FY 1981 - 9.4%, FY 1982 - 5.3%, and FY 1983 - 3.4%. Generally the cost estimate is completed two fiscal years prior to the budget year, which is the year design and construction will start. Consequently, in order to determine the cost of the project at the time of the actual construction the estimate must be escalated through those two years prior to the budget year and into the years in which the design and construction will take place.

60. What shortages or overages have occurred because of the differences in the estimated and actual escalation rates? How have these shortages or overages resulted in changes to the May 1980 estimate?

Answer: The overage due to the difference in the estimated and actual escalation is $938,000. The May 1980 estimate has not changed because actual escalation rates for FY 1984 and beyond are not known at this time.

61. How much of the project's $1,047,000 contingency remains?

Answer: The current cost plan reflects a current total contingency of $758,000 with approximately 90% of the procurement, installation and construction still uncommitted or uncompleted.

VII. ENERGY SCIENCE RESEARCH COMPUTATION (ESRC)

1. **The January 31, 1984 "Hollfield Tables" indicate that the IRB Fiscal Year 1985 budget request for the ESRC program totalled $53,460,000, including $48,610,000 for operating expenses and $4,850,000 for plant and capital equipment (PACE). According to these Tables, the Department's FY 1985 submission to OMB for the program totalled $54,145,000 including $49,295,000 for operating expenses and $4,850,000 for PACE. What are the specific differences between these two budgets?**

   Answer: The difference between the IRB and the OMB budgets is accounted for by the inclusion of program direction funds in the OMB budget for the ESRC program. The OMB budget for the ESRC program included $685,000 to administer this program. This request reflected an increase above the FY 1984 level and reflected the Department's desire to have the ESRC program established as a separate and independent organization within Energy Research. In the Internal Review Budget the program direction funds were provided for in other program budgets.

2. **Please provide detailed budget justifications for both the IRB budget and the Department's submission to OMB for the ESRC program proposed for FY 1985.**

   Answer: The Energy Science Research Computation request was $53,460,000 in the IRB, whereas the request to OMB was $54,145,000. This entire difference is accounted for by the inclusion of program direction funding of $685,000 in the request to OMB. The research request is therefore the same for each submission. The specific items requested are discussed on an activity by activity basis below.

   Supercomputer research in the amount of $42,610,000 in operating funds and $3,350,000 in equipment funds was requested, an increase of $27,940,000 over the FY 1984 level.

   Long Range Research in Supercomputing.....$24,610,000

   A total of $24,610,000, an increase of $10,140,000 over the FY 1984 level is requested for the Mathematical Sciences and Advanced Computing Concepts activities. This level will enhance the ongoing investigation of parallel architectures at several major universities and DOE laboratories, including the design and implementation of research machines for experimental studies.

   Experimental Computing Facilities.....$13,500,000

   A total of $13,500,000, an increase of $13,300,000 over the FY 1984 level, is requested for establishing and operating experimental computing centers based on new computer systems supplied by vendors.

   Supercomputer System Peripherals and Components.....$ 4,500,000

   In FY 1985, $3,000,000 will be used to initiate research on at least two candidate technologies for mass storage considered most promising for achieving a transfer rate of one billion bits per second by the end of the decade.

There is also a lack of a satisfactory archival (non-erasable and very low cost) storage system for long-term, high-volume storage of supercomputer results. An additional $1,500,000 will be used for research on archival storage techniques.

Capital Equipment.....$ 3,350,000

For FY 1985, $3,350,000 in capital equipment funds, an increment of $2,380,000 over the FY 1984 level, is requested to provide peripherals and network interface equipment for the experimental centers and the users of these experimental machines. Of these funds $1,100,000 will be used to upgrade the research computing facilities of the 11 DOE laboratories (including the NYU Courant Institute). The new centers will require $750,000 each to provide mass storage and network interface equipment for the experimental machines.

In the Energy Science Computation activity a total of $7,500,000 was requested. A total of $6,000,000 in operating funds was requested as a first step in expanding ER computing activities on the existing Magnetic Fusion Energy Computer Network into an overall Energy Research Computer Network to supply the large-scale computing needs of the High Energy and Nuclear Physics, Basic Energy Sciences and Biological and Environmental Research Programs.

Substantial data on the computing requirements of the Energy Research programs (with the exception of MFE) to be served by the network indicates that one additional state-of-the-art supercomputer system will satisfy those requirements in FY 1985. The costs associated with providing supercomputing resources for Energy Research scientists are as follows:

1. $3,500,000 for the lease and maintenance of the machine;

2. $1,500,000 for support staff to provide services for the broad spectrum of new users and applications;

3. $1,000,000 to expand the network communications and access facilities for these new users.

In addition, $1,500,000 in capital equipment was requested in this activity. Expansion of ER computing activities using the MFE Network to serve all Energy Research programs will require additional capital equipment for communications, peripherals and Remote User Service Stations. Specifically, $500,000 will be used for a hyperchannel and $400,000 for expanded disk storage. The remaining $600,000 will be allocated for communications equipment at selected energy research sites.

3. **Which portions of the proposed ESRC program were incorporated in the FY 1985 Applied Mathematical Sciences subprogram budget request?**

Answer: The Energy Science Research Computation (ESRC) request to OMB was $54,145,000 whereas the Congressional submission for Applied Mathematical Sciences is $29,750,000. The specific differences between these budget requests is explained on an activity by activity basis below.

The ESRC initiative to OMB included an increase of $10,000,000 for long range supercomputer research. The Applied Mathematical Sciences subprogram (AMS) request to Congress includes an increase of $6,580,000 for long range supercomputer research giving a total of $21,250,000 in this program. The ESRC initiative requested $13,500,000 operating funds and $3,350,000 capital equipment funds from OMB to support at least three Experimental Computer Facilities, incorporating vendor supplied mainframes with supporting research and development funds for operating systems, languages, etc. These mainframes would include new parallel architectures that show some promise of being the base of supercomputers of the future. The AMS subprogram request to the Congress has no funds for these facilities.

The ESRC initiative requested $4,500,000 from OMB to support research on high speed peripherals used with supercomputer systems. The AMS subprogram request to Congress has no funds for this research.

The ESRC initiative included $6,000,000 operating funds and $1,500,000 capital equipment funds from OMB for Energy Sciences Advanced Computation. The AMS subprogram request to Congress includes $7,000,000 operating funds and $1,500,000 capital equipment funds for this activity. The additional operating funds are included in the request to provide better network access to Energy Research contractors in universities and national laboratories.

DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
GEORGE E. BROWN, JR., CALIF.
JAMES H. SCHEUER, N.Y.
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TOM HARKIN, IOWA
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March 19, 1984

Alvin W. Trivelpiece, Director
Office of Energy Research
Department of Energy
Washington, D.C. 20585

Dear Dr. Trivelpiece:

The Subcommittee is continuing to evaluate the Department's fiscal year 1985 budget request for Supporting Research and Technical Analysis and High Energy and Nuclear Physics.

To facilitate this evaluation, I am enclosing several additional questions, in order to supplement the February 22 and 23, 1984 hearing record on these topics.

I would appreciate your responses to these questions by March 23, 1984 so that they may be received prior to full committee mark-up. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Wcw
attachment

EDA Subcommittee
Supplemental Questions

FY 1985 Authorization Hearings
Supporting Research and Technical Analysis
and
General Science and Research

1. On March 15, 1984 the Subcommittee on Energy Development and Applications approved language to be included in the Committee report on the "Department of Energy Civilian Research and Development Authorization Act for Fiscal Years 1985, 1986, and 1987," which in part says,

> "In view of the fact that the CEBAF facility is intended to perform experimental research at the frontier of modern science, it is essential that this effort be supplemented by an equally advanced program of theoretical and computational physics. This is true both during and after construction of the facility.
>
> For this purpose, the Department of Energy is directed to establish a state-of-the-art computer facility at a SURA university, with network access to the University of Virginia, the CEBAF site, and other involved SURA universities. The Committee believes that the existing proposal to the Department from a SURA university to establish such a center would serve as a basis for this activity."

a. Have you, in fact, received a proposal, prior to March 15, 1984, from a SURA university to establish a computer capability that could support this activity?

b. From which university?

c. Is this, as the Committee report language implies, the only such formal proposal the Department has received, as of March 15, 1984?

2. It is the Committee's intent that this existing proposal serve as the basis for establishing the required computer capability based at the proposing university.

a. Does the proposal contain cost-sharing provisions by the university? the state? the computer manufacturer?

b. Is the proposal broad enough to allow for the establishment of sufficient computational capability for the theoretical and computational physics needed by CEBAF?

c. Please explain how the center could be broadened to be integrated with the existing Department of Energy supercomputer access program.

d. Please explain how the facilities might be made available to DOE contractors for scientific and engineering purposes other than nuclear physics.

Questions and Answers

Relating To The

February 22, 1984

Hearing Before The

Subcommittee on Energy Development and Applications

Committee on Science and Technology

U.S. House of Representatives

Witness: Alvin Trivelpiece

Question: 1. On March 15, 1984 the Subcommittee on Energy Development and Applications approved language to be included in the Committee report on the "Department of Energy Civilian Research and Development Authorization Act for Fiscal Years 1985, 1986, and 1987," which in part says,

> "In view of the fact that the CEBAF facility is intended to perform experimental research at the frontier of modern science, it is essential that this effort be supplemented by an equally advanced program of theoretical and computational physics. This is true both during and after construction of the facility.
>
> For this purpose, the Department of Energy is directed to establish a state-of-the-art computer facility at a SURA university, with network access to the University of Virginia, the CEBAF site, and other involved SURA universities. The Committee believes that the existing proposal to the Department from a SURA university to establish such a center would serve as a basis for this activity."

a. Have you, in fact, received a proposal, prior to March 15, 1984, from a SURA university to establish a computer capability that could support this activity?

b. From which university?

c. Is this, as the Committee report language implies, the only such formal proposal the Department has received, as of March 15, 1984?

Answer: Yes, the Department, received a proposal for a SURA university to to establish a supercomputer center prior to March 15. The proposal was submitted by Florida State University. It is the only proposal received by the Department from a SURA university to establish such a computer center.

Question: 2. It is the Committee's intent that this existing proposal serve as the basis for establishing the required computer capability based at the proposing university.

a. Does the proposal contain cost-sharing provisions by the university? the state? the computer manufacturer?

Answer: The Florida State University proposal contains cost-sharing by the University, the State of Florida, and from a computer manufacturer.

b. Is the proposal broad enough to allow for the establishment of sufficient computational capability for the theoretical and computational physics needed by CEBAF?

Answer: The proposed supercomputer center at Florida State would provide the large-scale computing capability for engineering design studies and the theoretical and computational physics support needed for the CEBAF facility. In the early phases of CEBAF, engineering design would likely constitute the largest use.

c. Please explain how the center could be broadened to be integrated with the existing Department of Energy supercomputer access program.

Answer: The Department's supercomputer access program is intended to provide DOE contractors access to state-of-the art computing capability. Because of the difficulty of assembling a complete supercomputer system with the features required by users in diverse DOE programs, it will be some time before FSU or any new supercomputer center will be able to provide the quality, state-of-the-art service required. If in the future the FSU center became capable of providing quality service to SURA universities for nuclear physics, it could in principle, provide service to DOE projects in other fields at SURA universities. However, a decision to that effect could only be made after the capability of of the FSU center has been demonstrated.

d. Please explain how the facilities might be made available to DOE contractors for scientific and engineering purposes other than nuclear physics?

Answer: The proposed facilities FSU facility might be made available to SURA DOE contractors for scientific and engineering purposes other than nuclear physics by providing users access through the communications network which would be established to serve the SURA universities. As indicated in the answer to question 2c, assembling the complete system required to serve a diverse user group will require time, considerable effort and adequate financial support.

DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
GEORGE E. BROWN, JR., CALIF.
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U.S. HOUSE OF REPRESENTATIVES
COMMITTEE ON SCIENCE AND TECHNOLOGY
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February 28, 1984

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WILLIAM CARNEY, N.Y.
F. JAMES SENSENBRENNER, JR., WIS.
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Executive Director
ROBERT C. KETCHAM
General Counsel
DAVID S. JEFFERY
Minority Staff Director

Dr. George C. Pimentel
Associate Director
Lawrence Berkeley Laboratory
Berkeley, California 94720

Dear Dr. Pimentel:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

QUESTIONS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

DR. PIMENTEL

1. What is the scope of the study being conducted by the National Academy of Sciences/National Research Council (NAS/NRS) Committee to Survey Opportunities in the Chemical Sciences? When will the report be completed?

2. Does the proposed CAM program in catalysis address those research opportunities in chemical catalysis that you highlighted in your testimony?

NATIONAL RESEARCH COUNCIL
COMMISSION ON PHYSICAL SCIENCES, MATHEMATICS, AND RESOURCES
2101 Constitution Avenue Washington, D.C. 20418

COMMITTEE TO SURVEY
THE CHEMICAL SCIENCES

GEORGE C. PIMENTEL, CHAIRMAN
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALIFORNIA
BERKELEY, CA 94720

March 9, 1984

Honorable Don Fuqua
Chairman, Committee on
Science and Technology
U.S. House of Representatives
Suite 2321 Rayburn House Office Bldg.
Washington, D. C. 20515

Dear Mr. Fuqua:

Thank you for letting me testify before the subcommittee last February 23. I have shown several of my colleagues the proposed FY 1985 DOE budget for the Chemical Sciences. There was universal dismay among them that DOE might delay for a whole year exploiting the opportunities before us in chemistry that are directly relevant to the DOE mission. It was gratifying indeed to sense the responsiveness of your Committee to my urging that this delay be avoided if possible.

I am pleased to submit herewith answers to the questions addressed to me about my testimony. If there are any other questions, I would be pleased to respond.

Sincerely yours,

George C. Pimentel

George C. Pimentel, Chairman
Committee to Survey the
Chemical Sciences

Encl.

cc: Dr. Harlan Watson
Dr. William Spindel, NRC

The National Research Council is the principal operating agency of the National Academy of Sciences and the National Academy of Engineering to serve government and other organizations

ANSWERS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis
Testimony on February 23, 1984

1. What is the scope of the study being conducted by the National Academy of Sciences/National Research Council (NAS/NRC) Committee to Survey Opportunities in the Chemical Sciences? When will the report be completed?

ANS.: On the basis of the original Planning Committee's guidance, the Policy Committee agreed that the proposed survey should serve the following vital functions:

- o To display the array of exciting challenges in chemistry today
- o To enhance chemists' awareness of opportunities to address societal needs
- o To enhance societal awareness of its dependence upon chemistry for response to its needs and for amelioration of its problems
- o To strengthen the base for science policy decisions including funding priorities between and within disciplines
- o To consider the human and material resources needed to exploit the rich opportunities in chemistry both in the advance of human knowledge and in the increase of human well being.

To achieve these functions the report will be organized around target areas that display the current bounds of knowledge likely to be expanded and with the following specific emphases:

I. Intellectual Frontiers

- a. notable scientific advances during the last fifteen years;
- b. new and opening intellectual frontiers;

II. Response to Societal Needs

- a. notable applications during the last fifteen years;
- b. opportunities for response to present and future societal needs;

III. Techniques and Facilities

- a. special techniques, instrumentation, and facilities;

IV. Interactions with Other Fields

a. potential impacts and benefits to neighboring disciplines;
b. advances in other fields likely to impact on the area;

V. Resources Needed to Exploit Opportunities

a. Institutional: universities, federal laboratories, private research organizations, industries;
b. Human: education
c. Material.

The scope of the study being made by the Committee to Survey the Chemical Sciences extends over all of chemistry, including the areas that overlap contiguous disciplines. To illustrate, it includes the activities of research chemists who are helping advance the biotechnologies, of those who are learning how to monitor, and control environmental pollution, of those who are actively developing new materials of all kinds. The scope includes areas relevant to the excellent opportunities presently opening to chemical engineers but does not attempt to nor could it encompass all of that broad field. It is concerned mainly with the long-range, fundamental research frontiers, but with a definite preoccupation toward their potential for long range societal benefit.

It is hoped that the formal Survey Report will be completed and ready for public distribution toward the end of this calendar year, and surely in time for Congressional reference use in their consideration of the FY 1986 budget.

2. Does the proposed CAM program in catalysis address those research opportunities in chemical catalysis that you highlighted in your testimony?

ANS.: The subject of chemical catalysis extends over a number of subdisciplines: solution catalysis, surface catalysis, electrocatalysis, photocatalysis, and biological catalysis. The CAM program in catalysis does address some of these research opportunities, particularly in heterogeneous (surface) catalysis, as was evident in Dr. Somorjai's testimony.

George C. Pimentel

DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
GEORGE E. BROWN, JR., CALIF.
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COMMITTEE ON SCIENCE AND TECHNOLOGY

SUITE 2321 RAYBURN HOUSE OFFICE BUILDING
WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Albert Narath
Executive Vice President
Sandia National Laboratories
Albuquerque, New Mexico 87185

Dear Dr. Narath:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

QUESTIONS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

DR. NARATH

1. The ad hoc Panel Report recommended that the original NCAM materials initiative restate the goals and objectives to clarify the intended technology focus and Advanced Light Source (ALS) decoupling. What is meant by the term "technology focus"?

2. The ad hoc Panel recommended that construction of the Advanced Materials Synthesis Laboratory/Advanced Device Concepts Laboratory be deferred until a subsequent review of the NCAM program plan is available. What would constitute an appropriate review? When should it be done, and what criteria should be used to judge the acceptability of the program plan?

3. Who should perform this review? Should the same ad hoc Panel carry this out?

4. CAM's stated program objectives are "to perform high-quality, industrially responsive materials research, to educate the next generation of scientists and engineers, and to accelerate the translation of basic knowledge into new technology." Couldn't we best accomplish the first and third of these objectives by funding more basic research in which industry is the performer? What is the advantage of having a CAM involved?

A. Narath
Executive Vice President

Sandia National Laboratories
Albuquerque, New Mexico 87185

March 13, 1984

The Honorable Don Fuqua, Chairman
Committee on Science and Technology
U.S. House of Representatives
Suite 2321 Rayburn House Ofc. Bldg.
Washington, D.C. 20515

Dear Mr. Fuqua:

I appreciated the opportunity to appear before your Subcommittee on Energy Development and Applications at its Feb. 23, 1984 hearing. I have attached answers to questions raised in your letter of February 28, 1984, and would be happy to provide any additional information should that be needed to clarify my testimony.

Sincerely,

AN:tf

Attch.

1. The ad hoc Panel Report recommended that the original NCAM materials initiative restate the goals and objectives to clarify the intended technology focus and Advanced Light Source (ALS) decoupling. What is meant by the term "technology focus"?

   The "basic-research" mode of scientific inquiry has been motivated traditionally by human curiosity with little regard for the ultimate utility of the knowledge gained. Such pursuit of scientific opportunities has in the short span of a few decades created most of the fundamental knowledge upon which modern technology was built. There is also no doubt that future technological advances will require further additions to the knowledge base. Because of the speed of modern global communications, however, knowledge has taken on a ubiquitous character. Therefore, knowledge per se offers little competitive advantage to the nation producing it. It is now widely recognized that the key to success in international "high-tech" markets is superior ability in translating basic knowledge into new technology. In this context, "technology focus" refers to a structured research approach which is motivated by and directed toward a specific set of identified technological goals. Although U.S. basic science continues to excel, the pace of U.S. technological innovation frequently lags that of its competitors (e.g. Japan). This recent trend has resulted in a rapidly shrinking (or even reversing) margin of technological superiority in many areas. The Panel concluded that LBL with its outstanding program in the basic materials sciences is, in principle, well positioned to address this problem by directing future growth toward goal-oriented (i.e. "technology pull") efforts in a few strategically important materials areas.

2. The ad hoc Panel recommended that construction of the Advanced Materials Synthesis Laboratory/Advanced Device

Concepts Laboratory be deferred until a subsequent review of the NCAM program plan is available. What would constitute an appropriate review? When should it be done, and what criteria should be used to judge the acceptability of the program plan?

The intent of the recommended review prior to construction authorization of the AMSL/ADCL facility was to assure acceptable progress toward the establishment of additional research thrusts (i.e. in addition to the initial catalysis program) having the desired "technology pull" character. The review criteria should be based on the eight action items listed on pages 21-24 of the NCAM Panel's final report, especially in regard to program planning. Although not specifically discussed in its report, the Panel clearly had a rather formal review process in mind, in order to lend credibility to subsequent DOE decisions.

3. Who should perform this review? Should the same ad hoc Panel carry this out?

Although it is conceivable that the ad hoc Panel could be reconvened, DOE might prefer an independent review by a group of experts chosen specifically for this more narrow task.

4. CAM's stated program objectives are "to perform high-quality, industrially responsive materials research, to educate the next generation of scientists and engineers, and to accelerate the translation of basic knowledge into new technology." Couldn't we best accomplish the first and third of these objectives by funding more basic research in which industry is the performer? What is the advantage of having a CAM involved?

Significant opportunities for translation of basic knowledge into applications exist at established centers of excellence for basic research. Such centers exist at many universities, federally funded laboratories, and the major industrial research centers. It is doubtful, however,

that federal funding of industrial basic research for the purpose of technological stimulation is a wise investment since industrial programs are presumably already being managed to optimize the translation process at those locations. Universities and federal laboratories, on the other hand, have not participated to the same extent in that process and therefore offer in many cases outstanding opportunities for technological support. In addition, coupling the performance of basic research, graduate education and technology support in a single institution such as LBL promises (in principle, if not necessarily in practice) synergistic advantages not attainable in an industrial setting.

40-574 O - 85 - 61

DON FUQUA (Fla.), Chairman

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COMMITTEE ON SCIENCE AND TECHNOLOGY

SUITE 2321 RAYBURN HOUSE OFFICE BUILDING
WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Peter Eisenberger
Director of Physical Sciences Laboratory
Exxon Research & Engineering Company
Annandale, New Jersey 08801

Dear Dr. Eisenberger:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you and Dr. Knotek to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
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WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Michael L. Knotek
Surface Science Division 1134
Sandia National Laboratories
Albuquerque, New Mexico 87185

Dear Dr. Knotek:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you and Dr. Eisenberger to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

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QUESTIONS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

DR. EISENBERGER AND DR. KNOTEK

1. What are the relative advantages and disadvantages of the different types of synchrotron radiation sources such as soft x-ray, hard x-ray, and so forth?

2. Will synchrotron light sources currently operational or under active development really be oversubscribed by quality researchers by the end of this decade?

3. Your November 14, 1983 letter to Dr. Trivelpiece recommended the construction of a 6 GeV storage ring beginning in 1987, with R&D funding to be allocated in FY 1985 and FY 1986. What level of funding would you recommend in FY 1985 and FY 1986?

4. What is your estimate of the construction cost and operating cost of the 6 GeV facility?

5. Did DOE follow your recommendation, and request FY 1985 funding for the 6 GeV facility?

6. One line of argument goes as follows. First, the preferred 6-GeV storage ring is more costly than the ALS. Second, the 6-GeV machine needs much more R&D to reach the current level of maturity of the ALS design. Finally, it will take much longer to construct the higher energy device than the ALS. Given these factors, DOE should proceed with the immediate construction of the ALS.

   Are these arguments valid, and if so, are they sufficient reasons to proceeding with construction of the ALS now?

Sandia National Laboratories
Albuquerque, New Mexico 87185

March 14, 1984

Mr. Don Fuqua, Chairman
U.S. House of Representatives
Committee on Science and Technology
Suite 2321 Rayburn House Office Building
Washington, D.C. 20515
Attn: Dr. Harlan Watson

Dear Mr. Fuqua:

Dr. Eisenberger and I were delighted and honored to have the opportunity to give our testimony regarding our Planning Study for Advanced National Synchrotron Radiation Facilities to your Subcommittee. Attached are the answers to the supplemental questions which the Subcommittee submitted to us.

If there are any further ways we can assist or inform you on this most important topic please contact us.

Sincerely,

Michael L. Knotek
Surface Science
Division 1134

MLK:sln

Encl.

ANSWERS TO QUESTIONS FROM THE U.S. HOUSE OF REPRESENTATIVES SUBCOMMITTEE ON ENERGY DEVELOPMENT AND APPLICATIONS

FEBRUARY 23, 1984

FROM

Dr. P. M. EISENBERGER and Dr. M. L. KNOTEK

Question 1: What are the relative advantages and disadvantages of the different types of synchrotron radiation sources such as soft x-ray, hard x-ray, and so forth?

Answer 1: It is the conclusion of our committee that the scientific and technological opportunities offered by the new generation of insertion device based synchrotron radiation sources are great in both the soft x-ray and hard x-ray regions of the spectrum. As our report explains, the physics of insertion devices and storage rings dictate that for optimum performance across the spectrum, two storage rings optimized for the soft and hard x-ray regions, respectively, are necessary. We recommend that over the ten year period we were asked to consider both machines be built. The two prime factors which govern their relative priority are:

1.There are no existing dedicated facilities where hard x-ray undulators can be developed, whereas some limited opportunities for developing soft x-ray undulators do exist.

2. Although the soft x-ray ring cannot provide undulator capability in the hard x-ray region, the hard x-ray ring can access some of the soft x-ray region, albeit with reduced performance.

Question 2: Will synchrotron light sources currently operational or under active development really be oversubscribed by quality researchers by the end of this decade?

Answer 2: The report on the "Current Status of Facilities Dedicated to the Production of Synchroton Radiation" (The Lynch Report), published in 1983, concluded that user demand sould saturate capacity by 1985. While the primary motivation for the actions recommended in our report is the creation of new opportunites in science and technology rather than the creation of added capacity, we found that indeed the Lynch Report projections seem to be valid. The NSLS VUV-ring bending magnet ports are fully subscribed, and no more than four ports remain open on the x-ray ring. The SRC is approximately 70% committed even before becoming operational, and SSRL remains heavily oversubscribed. The quality of the research is reflected in the fact that allocation of beamtime and awarding of beamlines for Participating Research Teams is done on a competitive basis, and numerous groups have been turned away. The development of available straight sections with insertion devices will provide some advanced capability which is expected to be quickly saturated by cutting-edge efforts.

Question 3: Your November 14, 1983 letter to Dr. Trivelpiece recommended the construction of a 6 GeV storgae ring beginning in 1987, with R&D funding to be allocated in FY 1985 and FY 1986. What level of funding would you recommend in FY 1985 and FY 1986.

Answer 3: Current perceived needs by the institutions carrying out this research and development are ~ $1.25M in FY 1985 and $1.25M in FY 1986.

Question 4: What is your estimate of the construction cost and operating cost of the 6 GeV facility?

Answer 4: We have asked the institutions who plan to submit proposals for a 6 GeV ring to provide us with their current best estimates for the construction and operating costs for their proposed facilities. Their answers, together with some remarks on the relative capabilities to be provided by each facility are(in FY84 M$):

	Construction	Operating	Comments
Stanford:	168	25	10 beamlines, injector
Brookhaven:	150-200	30	10 beamlines, injector
Cornell:	60	5-7.5	10 beamlines, existing injector

It must be emphasized that these are rough estimates which have not been reviewed, and represent facilities with significant differences in detail.

Question 5: Did DOE follow your recommendation, and request FY 1985 funding for the 6 GeV facility?

Answer 5: We have no knowledge of funding by DOE specifically for R&D towards the 6 GeV ring. There are, however, efforts in design R&D at several facilities which are being carried out using existing funds. At this point there has not been a prioritization of the R&D areas by which to judge R&D proposals.

Question 6: One line of argument goes as follows. First, the preffered 6-GeV storage ring is more costly than the ALS. Second, the 6-GeV machine needs much more R&D to reach the current level of maturity of the ALS design. Finally, it will take much longer to construct the higher energy device than the ALS. Given these factors, DOE should proceed with the immediate construction of the ALS.

Are these arguments valid, and if so, are they sufficient reasons to proceeding with construction of the ALS now?

Answer 6: Regarding the first point, the 6 GeV ring must certainly be expected to cost more than the ALS; just how much more is a function of the design and is still under study (see the answer to question 4). Regarding the second point, the 6 GeV ring will require some R&D and design work before it reaches the maturity of the ALS; again we are not yet certain of the time that will ultimately be required. And on the final point, the time of construction will be a function of the size of the available design, engineering, and construction teams for the facility. Given that the facility will be physically 3 to 4 times the size of the ALS and will probably require construction of a building, one could reasonably expect a longer time for construction.

The three taken together are not reasons to proceed per se, but are among many other factors to be weighed in making the final decision. These points were all known by the committee when it made its recommendations, and therefore don't change our priority order. Our recommendations simply put are that an ALS type machine should be built at this time only with the confidence that it would not delay the implementation of the high energy ring. Without this confidence we would recommend that the 6 GeV ring be built first, followed by the earliest possible construction of the ALS type machine.

DON FUQUA (Fla.), Chairman

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COMMITTEE ON SCIENCE AND TECHNOLOGY

SUITE 2321 RAYBURN HOUSE OFFICE BUILDING
WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Hermann Grunder
Associate Director
Lawrence Berkeley Laboratory
Berkeley, California 94720

Dear Dr. Grunder:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you and Dr. Somorjai to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

* DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
BRUCE F. VENTO, MINN.
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[illegible], TENN.
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COMMITTEE ON SCIENCE AND TECHNOLOGY

SUITE 2321 RAYBURN HOUSE OFFICE BUILDING
WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Gabor Somorjai
Center for Advanced Materials
Lawrence Berkeley Laboratory
Berkeley, California 94720

Dear Dr. Somorjai:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you and Dr. Grunder to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

Lawrence Berkeley Laboratory
1 Cyclotron Road Berkeley, California 94720
(415) 486-4000 • FTS 451-4000

March 6, 1984

RECEIVED
MAR - 8 1984
COMMITTEE ON SCIENCE
AND TECHNOLOGY

Chairman Don Fuqua
U.S. House of Representatives
COMMITTEE ON SCIENCE AND TECHNOLOGY
Suite #2321, Rayburn House Office Building
Washington, D.C. 20515

Dear Mr. Fuqua:

It was a pleasure testifying before the Subcommittee on Energy Development and Applications on February 23, 1984, and we very much appreciate your continuing personal interest in the Laboratory's Center for Advanced Materials. Enclosed are our answers to the questions that you sent us subsequent to our testimony.

During the past week we have been in daily contact with DOE's Basic Energy Sciences program managers to provide information about CAM that would enable them to respond to questions from your Subcommittee staff. To the best of our knowledge, questions 1, 2, 5, and 7-39 of the package of questions sent to us are identical to questions being asked of the DOE. As a result, the enclosed answers to these questions are essentially the same as those being provided by the DOE, as they represent the Laboratory's and the Agency's considered positions. Questions 3, 4, and 6 are unique to our testimony.

We know of your keen interest in science education and hope that the answer to question 6 clears up any uncertainty in your mind regarding the unique educational opportunities possible via CAM.

Sincerely,

Hermann A. Grunder

Hermann A. Grunder
Deputy Director,
General Sciences

Gabor A. Somorjai

Gabor A. Somorjai
Catalysis Program Leader,
Center for Advanced Materials

HAG:gf
Encls.

QUESTIONS FOR DR. GRUNDER AND DR. SOMORJAI

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

1. **What is unique about CAM's mission "As an experiment in collaboration between industry and a federal laboratory"? Such collaboration has occurred in other laboratories, such as Oak Ridge, for example.**

   Uniquely, CAM includes as major participants in its programs visiting scientists from industry and academia along with graduate students, postdoctoral fellows, faculty members, and staff scientists.

   At a time when science education is a critical matter for national policy, CAM harnesses one of our nation's strongest centers for scientific education to meet industry's needs for materials scientists. Hence, the University connection and educational function of CAM yields a different form of collaboration between a Laboratory and industry.

2. **What "novel methods of cooperation and technology transfer between a federal laboratory and industry" is CAM exploring?**

   A major method is the establishment of industrial fellowships at CAM. Scientists from industry will work at LBL on CAM projects for a period of 3-12 months. They will bring industrial know-how to the CAM team and will return to their employer with new knowledge of methodology and basic scientific findings in their field. It can be expected that these fellows and their employers will then apply this knowledge to technological applications. In addition, the perspective of these industrial fellows will be a major stimulent to CAM graduate students, who are likely to go on to pursue industrial careers.

   Also, the total concept wherein industry directly relates to CAM through workshops and direct input on proposed research programs, is indeed, novel. Further, CAM has established a Scientific Policy Board reporting directly to the LBL Director composed of:

   John L. Doyle, Chairman
   Vice President, Research and Development
   Hewlett-Packard Company

   J.C. McGroddy
   Director, Organization Planning
   IBM

   Harold W. Paxton
   Vice President, Research
   United States Steel Corporation

J.R. Thomas
President, Chevron Research Company

John R. Whinnery
University Professor, U.C. Berkeley
Department of Electrical Engineering and Computer Sciences

Such oversight and guidance is also distinctly novel.

3. **On page 6 of your statement, you mentioned that "Industry is pledging money to support specific CAM programs." What amount of money is involved? Which companies are providing this support, and what programs are being supported?**

One of the policy questions that the CAM Policy Board will be considering has to do with the mechanisms and appropriate levels of industry involvement in CAM. Although formal solicitation has not yet taken place with respect to industrial support of CAM programs, the E.I. Dupont Corporation has offered $20,000 in support of CAM's catalysis program.

4. **Your testimony indicated that there was an industry participation workshop held on May 23, 1983. Was there a report published on this workshop, and if so, please provide several copies?**

Ten copies of the Report of the Industry Workshop, Lawrence Berkeley Laboratory, May 23, 1983, PUB-5101, are enclosed.

(Note: This report is reproduced in Appendix II.)

5. **LBL's MMRD trains hundreds of graduate students. What will CAM do to educate and train people in the materials sciences that the MMRD could not do with equivalent resources?**

CAM differs substantially in intent from MMRD. Both involve research conducted at the fundamental end of the research and development spectrum of advanced materials technologies. However, each CAM program includes several investigators engaged in a focused activity, whereas MMRD conducts research on an individual investigator basis and without the explicit industrial interaction required for CAM programs. Also, CAM graduate students will have the opportunity of working with industrial Fellows on industry related technology.

6. **In your oral testimony you indicated that LBL wants the graduate student population to grow to 600. What commitments do you have from the University of California that additional faculty will be available at the Berkeley campus to handle this upsurge in the number of graduate students?**

The Lawrence Berkeley Laboratory presently involves at least 540 graduate students in its programs, 360 of these in MMRD. The figure of 600 graduate students mentioned in my testimony is for both the MMRD and CAM program areas. With the start up funding of $2.9 million in FY 1984, the CAM program will involve 44 graduate students. Because these are new programs, the number of graduate students will not increase proportional to funding, but will be limited to approximately 240 students when the Center is fully operational. Discussions and negotiations with department heads at the Uni-

versity have established the feasibility of reaching this level of student involvement in CAM within the present general campus-wide plan.

7. **The MMRD is interdisciplinary. Why can't the MMRD be utilized in much the same way as the National Science Foundation's Materials Research Laboratories to developed focused, interdisciplinary materials research programs?**

MMRD is a major national asset, but its personnel and organization are not designed for the mission envisioned for CAM. MMRD has become one of the world's most successful materials and chemical sciences research units by providing stable support for and encouraging interactions among principal investigators who pursue research topics of their choosing assisted by post-doctoral scientists and graduate students. Some of MMRD's most successful and productive contributors to the advancement of basic science would be unsuited to the more focused programs and management of CAM. CAM is designed as a home for focused, large team basic research carried out in close interaction with industry. Interactions between MMRD and CAM with their different perspectives and goals, but similar drive for excellence and well-trained, high-caliber scientific staff should contribute in a significant way to the nation's material science research objectives.

8. **CAM's stated objectives are "to perform high-quality, industrially responsive materials research, to educate the next generation of scientists and engineers, and to accelerate the translation of basic knowledge into new technology." Couldn't we best accomplish the first and third of these objectives by funding more basic research in which industry is the performer? What is the advantage of having a CAM involved?**

CAM's program objectives should not be considered separately from the institutional setting provided by Lawrence Berkeley Laboratory as a DOE national laboratory.

The Office of Energy Research has responsibility for policy guidance as well as substantial programmatic direction for the non-weapons multiprogram laboratories of the Department. There has long been concern that the missions of these laboratories be more responsive to changing requirements, and that their research as well as their facilities become more available and relevant to industrial needs. It is a situation that requires continuing oversight as the requirements of the Department and national needs evolve. The recent reports by the ERAB and the Packard Panel are examples of this oversight.

With this in mind the decision was made to build on the demonstrated research excellence in the basic materials and chemical sciences at LBL. Unique among the national labs was the laboratory's strong connection to and interaction with the faculty and graduate students of the University of California at Berkeley. What CAM adds to this is a programmatic, focussed effort on research established with the advice of industry, and within which industrial collaborators are intended to play a role more intrinsic than being simply users.

CAM's objectives are also interrelated and should not be considered independently. For example, transferring basic knowledge into new technology happens best by providing industry with minds trained with state-of-the-art

equipment on frontier research problems. Traditionally, however, university research is driven by its own internal imperatives. The establishment of CAM at LBL includes the imperatives of industry as well so that the basic research pursued results in skills and knowledge more immediately useful to industry.

In general, industry's basic research efforts are much more targeted than CAM's are intended to be. Research areas are often extremely narrow to correspond with specific market opportunities, and the resource base of manpower and disciplines available in most industrial laboratories is not nearly as broad as that now available at national laboratories. If the federal government were to broaden its direct support of industry's basic research, several difficulties could arise. Building the breadth and depth required for pursuing the activities envisioned for a CAM at a single company would require an investment of at least the same magnitude as CAM. Even if the investment were spread among several companies, productive use of funds would require that those companies already have a "critical mass" of research and manpower. Companies with that level of investment in research usually have dominant market positions. Thus, federal assistance must be judicious, indeed, to avoid either the perception or reality of anticompetitiveness.

9. **How much funding will the Electronics Materials Program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment.**

Operating expenses are $600,000 for FY 1984 and $740,000 for FY 1985.

The equipment budget is not subdivided by programs since major instruments and equipment are used on more than one program. The total equipment funding for CAM is $1,200,000 for FY 1984, $600,000 for FY 1985. A solid state Nuclear Magnetic Resonance unit and a Fourier transform I-R Spectrometer are examples of instruments that will be used on more than one program.

10. **Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.**

FY 1984:

An interim crystal growth Laboratory is being installed with the necessary materials handling equipment.

Specifically, two Bridgman crystal pullers, 3" and 5" diameter, are under procurement and will be operational by August/September 1984.

A numerical modeling program for heat and mass flow during crystal growth has been fully developed and tested; and it will be adapted to the Bridgman technique to calculate heat flow, temperature distribution, and thermal stresses.

Doping experiments specifically aimed at dislocation reduction.

A research program for the expansion of Lang topography of dislocations in GaAs using synchrotron radiation at SSRL is under development in collaboration with staff at Hewlett-Packard Laboratories.

A new Electron Paramagnetic Spectrometer is under procurement. This instrument will play a crucial role in the identification and the exploration of the structure of defects in GaAs, specifically the antisite defect.

A far infrared Fourier transform interferometer shared by many CAM programs will shortly be purchased for the study of shallow and deep level defects in bulk single crystals and thin films of GaAs.

The Atomic Resolution Microscope (ARM) at LBL's National Center for Electron Microscopy is presently being used to obtain the first atomically resolved pictures of the GaAs lattice.

FY 1985:

Start-up of routine GaAs crystal growth.

Characterization methods developed and adapted in FY 1984 will be used for the in-house-grown crystals and will provide direct feedback to improve growth parameters.

First results from detailed defect studies (such as EL2) can be expected.

Numerical finite element analysis will be applied to natural convection problems in the melt of the crystal puller.

MBE facility at the Department of Electrical Engineering will be expanded to a state-of-the-art, three-chamber system.

FY 1986:

Crystal purity will be pushed to higher limits. Study of the purity of starting materials, crucibles, and ambient gases together with advanced high-energy SIMS analysis, IR-spectroscopy, EPR and x-ray fluorescence of the GaAs bulk materials will lead to an identification of the major impurity sources.

The state-of-the-art MBE facility will permit growth of epitaxial films on in-house-grown GaAs substrate. This will permit the study and control of defect and impurity interaction between bulk substrate and epilayer.

Collaboration with device manufacturers using CAM GaAs will lead to first definitive results on defect-device performance correlations.

The availability of adequate space is a most important issue for the success of the Electronic Materials Program of CAM. During the start-up phase FY 1984 and FY 1985 it will be possible to utilize laboratory space on the U.C. campus and in existing buildings at the Lawrence Berkeley Laboratory. As the program grows new special space requirements will become crucial. Clean room facilities which are standard for advanced semiconductor work will be needed. Crystal pullers of two to three stories height will have to be accommodated in the new AML building. Clean room, crystal growth equipment and materials preparation facilities must necessarily be co-located. The total space requirement is estimated at approximately 20,000 feet, 16,000 square feet of which would be laboratory space and the rest, 4,000 square feet, would be office space for staff, visitors, and industrial fellows.

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11. What unique physical properties of gallium arsenide will CAM explore that other ongoing research within DOE, other agencies such as NSF and DOD, and industry are not exploring? What is the uniqueness of the CAM program?

The uniqueness of the CAM Electronic Materials program lies in the joining of a number of the best scientists and engineers of a National Laboratory, a leading University Campus and several companies from throughout the nation to solve the scientific problems which impede the development of advanced high speed, low power consumption devices, electro-optic devices, high speed sensors and digital converters. Initial emphasis is on the growth and characterization of large (greater than 7 1/2 centimeters), single crystals of gallium arsenide which, at present, is not being addressed in this country.

Some physical properties to be studied are:

Critically resolved shear stress at elevated temperatures of single crystals.

Morphology and stability of interfaces between liquid and solid GaAs during crystal growth.

Convection in GaAs melt and in growth ambient.

Real space and electronic structure of the most important shallow and deep level defects.

Defect and impurity interaction between bulk substrate and epitaxial layer.

12. What is the "track record" of the CAM investigators participating in the production, processing, and other aspects of the gallium arsenide research program?

The initial CAM Electronic Materials Team includes:

W. Hansen (LBL) and E. Haller (LBL and UCB) have successfully grown the world's purest semiconductors for use in nuclear radiation detector application.

B. Rubinsky (LBL and UCB) is one of the most successful young theorists in the application of front-tracking finite element analysis.

E. Bourret (LBL) is a leading expert in the theory and the experiment of compound semiconductor crystal growth. She recently joined CAM, coming from M.I.T.

P. Richards, E. Weber, P. Yu (all LBL and UCB) are leaders in IR-spectroscopy, deep level studies and pico-second spectroscopy respectively.

R. Gronsky (LBL and UCB) is one of the world's most outstanding electron microscopists. He is in charge of the atomic resolution microscope at NCEM.

D. Hess and S. Wang (both LBL and UCB) are thin film and epitaxy specialists with experience in industry (Hess) and academic research.

N. Cheung (LBL and UCB), J. Jaklevic (LBL) and N. Amer (LBL) are leading experts in structural and electronic properties and analysis using Rutherford Backscattering Spectrometry (RBS), x-ray topography and novel technique photothermal imaging.

13. How much funding will the polymer and polymer composites program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment. What arrangements are being made to take advantage of the unique equipment and facilities at Lawrence Livermore National Laboratory that may be applicable to this program?

Operating expenses are $360,000 for FY 1984 and $450,000 for FY 1985.

Capital equipment is not subdivided by program since major instruments and equipment are used on more than one program. The total equipment funding for CAM is $1,200,000 for FY 1984, $600,000 for FY 1985. A solid state Nuclear Magnetic Resonance unit and a Fourier transform I-R Spectrometer are examples of instruments that will be used on more than one program.

CAM researchers met in December with John Kolb and Richard Christensen from the Composites and Polymers Technology Group at Lawrence Livermore National Laboratory (LLNL) to discuss areas in which the two facilities might interact. LLNL expertise is heavily oriented towards structure/properties work, while CAM research is focused on processing science. The two programs are complementary. LLNL production and development responsibilities are expected to provide the same kinds of stimuli to CAM processing research as the inputs from more traditional industrial laboratories. LLNL synthesis capabilities could be helpful for specific synthesis needs in the future, but industrial sources are currently more appropriate.

The CAM Polymer and Polymer Composites program currently utilizes laboratory space in the College of Chemistry on the UCB campus. This space is filled to capacity and currently there are no facilities in close proximity for industrial fellows, or divisional fellows.

The industrial workshop recommendation called for developing synthesis, structure determination, and structure/properties expertise in order to meet program objectives. This cannot be done in the absence of additional facilities. Space in the proposed AML building of approximately 20,000 square feet - 75% devoted to laboratory space including adequate fume hood and chemical synthesis and analysis facilities will be required if the program is to meet the long term objectives as outlined in the Program Discussion Document and discussed at the industrial workshop.

14. Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.

MILESTONES

FY 1984

Begin spectral measurements and rheological characterization of polymer liquid crystals.

Measure flow fields and fiber orientation in fiber filled composites flowing through contractions.

Begin rheological characterization of block copolymers.

Elucidate phase compositions of polymer-solvent-nonsolvent systems.

Initiate theoretical activity and numerical modeling to support all experimental efforts.

FY 1985

Begin NMR characterization of polymer liquid crystals at various levels of deformation in Mechanical Spectrometer and capillary rheometer.

Begin measurement of rheology of polyester/glass fiber/small particulate systems.

Continue rheological characterization of block copolymers.

Obtain data on velocity field for a single fluid flowing around a sharp corner and two immiscible co-current fluids flowing in a straight channel.

Complete programming of finite-element computation for co-current flow.

Prepare membranes under well controlled conditions and examine membrane morphology.

Complete measurements of fiber orientation and kinematics in contraction and compare with finite-element calculations using continuum theory.

Develop strategies for molecular weight and composition distribution control in copolymerization.

Design and construct optical system for rheogoniometer, to detect and measure the characteristics of microstructures found in shear and of those formed at equilibrium but then deformed.

Incorporation of realistic temperature-dependence in all parameters in final theory of microphase separation, and evaluation of model predictions.

Begin new theory of block copolymer melt rheology.

Perform yield-stress measurements with new device, on selected block copolymer melt samples.

FY 1986

Obtain data on velocity field and interface location for two immiscible fluids in co-current flow around a sharp corner. Examine effect of viscoelasticity, and compare results to finite-element computations.

Continue NMR characterization of structure development with deformation in liquid crystal polymers.

Complete rheological characterization of polyester/glass fiber/small particulate systems without crosslinking, and begin study of cross-linking systems.

Begin theoretical study of spatial development of discontinuities (domains) in Leslie-Ericksen liquid crystal theory.

Begin theoretical and experimental studies on the influence of solvent-nonsolvent on the morphology evolution in block copolymers and polymer blends.

Complete the microstructural theory of block copolymer melt rheology.

Perform rheogoniometer measurement on selected block copolymers to obtain linear and non-linear fluid properties while recording microstructural information with the optical system. Supplement flow data with solid-state characterization of the same samples by electron microscopy and, if available, also by SAXS.

15. **How will the CAM polymer and polymer composites program complement, supplement, or duplicate research being conducted at the Polymer Processing Center at the Massachusetts of Technology, the University of Massachusetts-Industry Program on Polymers, and the Center for Applied Polymers at Case Western Reserve University? How many of the industrial sponsors of these centers were consulted in the development of the CAM program in this area?**

The CAM workshop on the program in Polymers and Polymer Composites was attended by representatives of ten major polymer producers and processors, including Dupont, Dow, Celanese, Boeing, Ford, and IBM, as well as representatives from small companies and research laboratories. Most companies represented participated in one or more of the programs at M.I.T., University of Massachusetts, and Case Western Reserve, and in several cases of which we are aware, it was the corporate representatives to these programs who attended the CAM workshop. Numerous other polymer producers and processors were also consulted during the formative period of the program. An advisory group is currently being organized with membership from Dupont, Celenese, IBM and Dow.

The CAM program largely complements the programs at M.I.T., Massachusetts, and Case Western Reserve. As discussed in the response to Question 17, the CAM program focuses on the basic science underlying processing technology in order to develop predictive ability for microstructure distribution. The M.I.T. program focuses on the solution of particular engineering problems related to applications; in an industrial context, it represents the type of research that one might expect to find in the research laboratories of an operating division rather than in a central research laboratory. The University of Massachusetts program emphasizes polymer synthesis and characterization, while the Case Western Reserve program emphasizes structure determination. These are clearly "broad brush stroke" descriptions, and there are elements of all aspects in all programs, but the differences in complementary emphases are real and important.

16. How will the CAM polymer and polymer composites program complement, supplement, or duplicate research being conducted in other DOE-sponsored research programs in this area, including Defense Programs and the Advanced Gas Centrifuge Program, as well as other agency-sponsored programs? How many of these other-agency and other-DOE researchers were consulted in the development of the CAM program in this area?

Polymer and polymer composite research is funded by several of the offices of DOE. Except for the fundamental research funded by Basic Energy Sciences, the research is applied, highly specific to certain materials and applications. The CAM research program complements and extends the polymer research funded by Basic Energy Sciences. The topics in CAM were chosen to avoid unnecessary duplication. The National Science Foundation funds research in polymers in the areas of fundamental behavior of synthetic macromolecules; synthesis of new high molecular weight polymers with precisely defined structures; characterization of chemistry and structure of polymers; molecular arrangements in amorphous and crystalline polymers and mixtures; macromolecular chain dynamics and relaxation, molecular characteristics and their relation to mechanical, optical, transport, surface, and solvent properties; and theoretical treatment of macromolecular behavior. Industrial research in polymers is extensive; however, a large number of industrial consultants were involved in the definition of the CAM program to insure that the research would not duplicate the industrial effort. (See answer to Question number 15.)

Examples of research funded by DOE in polymers and polymer composites are given below by Office.

Conservation and Renewable Energy:

- Electronic and ionically conducting polymers and battery applications and electrotypic cells.
- Fiber reinforced composites for prototype fly wheels.
- Polymers for energy storage.
- Polymeric solar collectors and cover plates.
- Polymeric seals and gaskets.
- Polymeric membranes for low energy separations.

Military Applications:

- Surface chemistry and bonding of polyaramid fiber reinforced composite.
- Effect of crosslink density on toughness of rubber-modified epoxies.
- Creep-rupture and failure of Kevlar reinforced composites.
- Conducting polymer for electrode materials for high power density batteries and fuel cells.

- Water vapor permeation through elastomer films.
- Super-hard parylene polymer coating development and loading of high-Z metals.
- Low density, microcellular polyolefin foams.
- Evaluation and testing of commercial polymers and adhesives for weapons programs.
- Injection mold process for carbon-fibre reinforced snap-on fittings.
- Composite spring support structures.

Uranium Enrichment and Assessment

- Assessment of commercially available rotor materials for advanced gas centrifuge (test results and materials are classified Restricted Data).

Basic Energy Sciences

- Membrane separations.
- X-ray and neutron scattering to determine polymer structures.
- Degradation and bonding in silver/polymer solar materials.
- Probabilistic models of the stress-rupture of composite materials.
- Analysis of failure modes in short fiber reinforced thermoplastics.
- Structure-property requirements of polymers in mechno-chemical systems.
- Synthesis of water-soluble copolymers and polymers for enhanced oil recovery.
- Corrosion resistant polymer coatings.
- Photophysical studies in pure polymeric films.
- Dynamics of molecular orientation and relaxation in polymers.
- Polymeric ionic and electronic conduction.
- Rubber elasticity.
- Microstructural analysis of ion containing polymers.

17. What unique physical properties of polymer and polymer composites are being measured or explored that other ongoing research is not exploring? What is the uniqueness of the CAM program?

The CAM polymer and polymer composites program is not measuring or exploring unique physical properties of any material, although physical property measurement and prediction is an essential component of the program. The CAM program focuses on the generic problem of predicting microstructure and microstructure distribution during processing in the fluid state. The general problem requires incorporation of complex fluid rheology, equilibrium thermodynamics, and phase transition kinetics with a description of system geometry, fluid mechanics, heat transfer, mass transfer, and even aerodynamics in the analysis of processing steps such as compression or injection molding and fiber and film extrusion. One example is the prediction of the statistical fiber orientation distribution function and matrix residual stress in the molding of short-fiber polymer composites.

There is general agreement among industrial practioners, reinforced by the participants at the CAM Polymer and Polymer Composites workshop in October, that there is a pressing need for basic research in the science that underlies advanced polymer and polymer composite processing in order to achieve predictive ability regarding microstructure formation. Such research is not carried out extensively in industry, nor is it a primary focus of the programs mentioned in Question 15. It is this focus on basic processing science that makes the CAM program unique.

18. What is the "track record" of the CAM investigators participating in the production, processing, and other aspects of the CAM polymer and polymer composites program?

Program leader Morton M. Denn has been active in research in polymer processing and rheology for nearly twenty years, during which time he has been an active consultant to major polymer producers and processors. He is the author of four books, numerous book chapters and review papers, and seventy technical papers; more than half of these publications are on subjects relevant to the current CAM program. He is on several major editorial boards. In addition to his industrial consulting, his recognition by industrial practitioners includes the invitation to present the principal lectures at the Third Fiber Producer Conference in 1983. He has been a Guggenheim Fellow (1971-1972) and a Fulbright Lecturer (1979), and presented the William N. Lacey Lectures at Cal Tech in 1979 and the Peter C. Reilly Lectures at Notre Dame in 1980. He was awarded the Professional Progress Award from the American Institute of Chemical Engineers in 1979 "for his incisive investigations into polymer processing and his pioneering studies into process dynamics and control." He has held a Visiting Senior Lecturer position at M.I.T. since 1978, and he was the Visiting Chevron Energy Professor at Cal Tech in 1980.

David S. Soong has been a faculty member at the University of California since 1979 and was promoted to Associate Professor with tenure in 1983. During that time he has published over thirty technical papers on subjects relevent to the CAM program. He is an industrial consultant and a member of the Editorial Advisory Board of the Journal of Polymer Science.

Jeffrey A. Reimer joined the University of California after receiving a Ph.D. in Chemistry at Cal Tech and spending two post-doctoral years at the IBM T.J. Watson Research Center. He is a specialist in Nuclear Magnetic Resonance Spectroscopy, and he was published sixteen technical papers. He was an invited speaker in 1981 at the meeting of the American Physical Society and the 9th International Conference on Liquid and Amorphous Semiconductors.

Michael C. Williams, also on the faculty of the University of California, has been active in research in polymer science and engineering for more than twenty years. He is the author of ninety research papers, approximately two-thirds of which are on subjects relevant to CAM research. He has consulted for industry.

19. **Several programs in DOE, including the Materials Sciences subprogram and the Energy Conservation Program, as well as NASA, NSF and other agencies and industry are funding a considerable amount of R&D in ceramics. How does the CAM ceramics program relate to (1) other DOE and other agency ceramics research, and (2) to industrial ceramics research?**

The U.S. research programs in ceramics, funded from all sources, are numerous and varied. DOE/BES alone funds over 100 different ceramic research projects. Common to all of the programs concerned with ceramic processing and high temperature mechanical properties evaluation is the need to broaden their fundamental scientific base. Some large programs, such as those involved in the development of specific ceramics for engines, sponsored by NASA and by DOE/Conservation, have mainly ceramic development of ceramic engine demonstration objectives. In their research aspects, they aim at providing a fundamental technology base. The CAM ceramics program, however, seeks to develop a fundamental science base. Thus, the CAM ceramics program complements such programs by addressing fundamental questions of a more generic nature. It aims to transfer rapidly and effectively the knowledge that it generates in the first instance to the community developing the technology base for the fabrication of reliable advanced structural ceramics, such as those needed for the novel engines. The CAM ceramics program seeks interaction with, and offers the possibility for these industries to influence substantially the scope and direction of the CAM-ceramics scientific program by participation on a Program Advisory Committee, by having participating Industrial Fellows, and by exchanging materials and personnel. Similar interactions are offered to the academic community.

20. **How much funding will the CAM ceramics program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment.**

Operating expenses are $240,000 for FY 1984 and $370,000 for FY 1985.

Capital equipment is not subdivided by program since major instruments and equipment are used on more than one program. The total equipment funding for CAM is $1,200,000 for FY 1984, $600,000 for FY 1985. A solid state Nuclear Magnetic Resonance unit and a Fourier transform I-R Spectrometer are examples of instruments that will be used on more than one program.

21. **Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.**

FY 1984:

Hold workshop for program development.

Initiate organization of fabrication facility.

Initiate examination of model colloids.

Initiate powder characterization studies.

Initiate multiparticle sintering work on 2-dimensional model powders.

Initiate examination of creep-damage on SIC.

FY 1985:

Installation of equipment in fabrication facility.

Examine settling behavior of model colloids by diffraction methods.

Fabricate silicon nitride powders by gas phase reactions.

Commence selective baseline study of state-of-the-art silicon nitrides and carbides.

Examine sintering stresses with loading dilatometer on model powders.

Initiate development and construction of high temperature-high pressure loading dilatometer.

Initiate work on high temperature damage model development.

Initiate work on high temperature erosion and wear experiment.

FY 1986

Continuation of work in FY 1985 and in addition:

Initiate installation of class 1000 cleanroom.

Complete construction of high temperature-high pressure dilatometer and initiate densification studies on silicon nitride.

Initiate study of effect of abrasive wear on high temperature mechanical behavior.

Develop theories on high temperature erosion and wear from observation of damage in elementary erosion and wear events.

The development of the full CAM-Ceramics program will require the coherent grouping of new laboratories and personnel. The new laboratories will house the powder fabrication and consolidation equipment, including a class 1000

clean room, new equipment for injection molding experiments, and erosion and wear equipment, as well as high temperature mechanical testing equipment. Space for additional personnel, including the Industrial and Academic Fellows, need to be located in close proximity with ongoing work. A coherent space of approximately 15,000 to 20,000 square feet, including about 1/5 of this as office space, is needed to house the steady-state CAM- ceramics program. Such a space should be provided in the new Advanced Materials Laboratory, since its inclusion in current LBL Laboratory complexes would cause a major disruption in the present active LBL programs.

22. **The CAM Workshop on Advanced Structural Ceramics, originally scheduled for December 1983 was cancelled. What is the basis for the ceramics program being initiated by CAM? How is this program based on specific materials-related "stopper" problems identified by industry?**

The CAM workshop, originally scheduled for December 1983 was postponed since a number of key individuals were unable to attend at that time. The workshop is now scheduled for April 12 and 13, 1984. The CAM ceramics program was deemed suitable, after an LBL and DOE/BES review, to be considered for inclusion in CAM, with a target starting date of February 1, 1984, and with a modest budget permitting further program refinement, development and initiation. The scope and approach of the CAM ceramics program has already been shaped as a result of extensive discussions with NASA and DOE/Conservation, as well as by various inputs from concerned industries. The incorporation of this input into the program plan is expected to make the April workshop more effective.

The CAM ceramics is not intended to operate on a task-force basis. As such, it will not directly address industrial "stopper" problems of a short-term nature. Rather, it provides crucial, long term, fundamental research needed to guide development of the next generation of advanced structural ceramics. The development of such a fundamental science base is currently not occurring at a sufficiently fast rate. It is a major cause for the loss of a strong internationally competitive technology position. This will not only require focussed efforts such as the CAM - ceramics program, but will necessitate involvement, collaboration and substantial expansion of the entire national ceramic research effort.

23. **How does the CAM ceramics program complement, supplement, or duplicate ceramics research being carried out at the Center for Ceramics Research at Rutgers University or at Oak Ridge National Laboratory? How many of the industrial sponsors of the Rutgers' Center or researchers at Oak Ridge National Laboratory were consulted as to the content of the CAM program in ceramics?**

Discussions concerning program scope and elimination of overlap were held with J. Wachtman, Director of the Rutgers Center, and with V. Tennery, Ceramic Program Director at the Oak Ridge National Laboratory. As a result of these discussions, any significant overlap of the CAM ceramics program with these programs has been eliminated, and possible avenues for collaboration, such as use of facilities and exchange of materials, have been explored. A close relationship exists in the Rutgers program dealing with powder fabrication methods. Rutgers is further exploring the laser processing of silicon nitrides and carbides. The CAM ceramics program will use RF generated plasmas to fabricate powders tailored to the program needs.

The workshop document, describing the CAM ceramics program in detail, was distributed to ranking members of 14 companies engaged in fabrication or use of high temperature structural ceramics. A number of these companies are also sponsors of the Rutgers ceramics industrial consortium. An opportunity was thus provided for program input.

24. What unique physical properties of ceramics are being measured or explored that other ongoing research is not investigating? What is the uniqueness of the CAM ceramics program?

The CAM ceramics program addresses fundamental scientific questions relating to ceramics fabrication, high temperature properties such as surface properties of ceramic powders, creep-damage accumulation, cyclic loading effects, and erosion and wear in corrosive environments. It explores these properties with a range of unique tools available at LBL, such as atomic resolution electron microscopy, various advanced surface characterization methods, and novel dilatometry techniques.

The CAM ceramics program brings together a group of investigators from different disciplines. It has the closest National Laboratory - University program interaction anywhere. A survey of the ongoing research on related subjects in the U.S. has led to a program formulation that minimizes overlap with other efforts.

25. What is the "track record" of the CAM investigators participating in the processing, production, and other aspects of the CAM ceramics program?

At present, four senior investigators are involved in the CAM ceramics program. A summary of their vitae is as follows:

1. Lutgard C. DeJonghe, Staff Senior Scientist at the LBL MMRD, and Associate Professor in Residence, Department of Materials Science and Mineral Engineering, UC Berkeley. Chairman, first Gordon Research Conference on Science of Ceramic Processing (1981). Editor DOE/BES/Bulletin "Ceramics Science of Processing". Editorial subcommittee American Ceramic Society, Electronics Division. Member American Ceramic Society, National Institute of Ceramic Engineers, Ceramic Education Council, Electrochemical Society. 52 refereed journal publications. 2 patents including one patent on a ceramic fabrication technique.

2. Anthony G. Evans, Professor of Materials Science, Department of Materials Science and Mineral Engineering, UC Berkeley, and Faculty Scientist, LBL, MMRD. Chairman Gordon Research Conference on Mechanical Properties of Ceramics (1978). Editor, Basic Science Division, American Ceramics Society. Associate Editor, Materials Science and Engineering. Member of committees of the National Materials Advisory Board, National Academy of Sciences, National Research Council. Member Materials Research Council Steering Committee. Fellow American Ceramic Society. Member American Institute of Metallurgical Engineers. 110 refereed journal publications.

3. Ian Finnie. Professor and Chairman of Mechnical Engineering Department, UC Berkeley, and Faculty Scientist, LBL, MMRD, National Academy of Engineering. Vice President, American Society of Mechanical Engineers. Guggenheim Fellow. Member Institute of Mechanical Engineers (London), American Society for Testing and Materials. 120 refereed journal publications.

4. Clayton J. Radke. Associate Professor Chemical Engineering, Chemical Engineering Department, UC Berkeley, and Faculty Scientist, LBL, NSF Senior Fellow. Member American Chemical Society, American Institute of Chemical Engineers, Society of Petroleum Engineers, American Rheological Society. 25 refereed journal publications.

26. A major initial thrust of the advanced surface instrumentation program is to develop a scanning tunneling microscope modeled after a prototype recently developed by IBM in Zurich. What workshops, consultations, etc. were held to choose this program? How is this program based on specific materials-related "stopper" problems identified by industry?

The program was initiated after detailed discussions with Binning and Rohrer (IBM Zurich), Wilson (IBM San Jose), Quate (Stanford University), Golouchenko (Bell Labs), and others. A workshop bringing together workers in this field may be held in the near future as needs warrant.

Surface phenomena are the source of industrial "stopper" problems in many areas, from chemistry and catalysis to electronic device development. A direct route to solving those problems requires understanding surface structure, and data obtained from the STM should help in this regard. Two examples of specific problems to be tackled early with the CAM STM are: First, an investigation of the surface properties of Electronic Materials, in close collaboration with the GaAs program, in an attempt to shed light on the difficulties of producing a satisfactory oxide layer. Second, a study of the reconstruction of surfaces, in collaboration with theoretical members of the program, in an attempt to understand the role of this process in the adsorption of surface layers and catalysis.

In addition to the scanning tunneling microscope, the program includes developing several other surface oriented instruments and techniques. Y.R. Shen is developing techniques to exploit the second harmonic generation of laser light by adsorbed layers on surfaces. The scattered light is a sensitive probe of such properties as the nature, coverage, orientation, and bonding of adsorbed molecules. The technique can be applied to surfaces in vacuum and also to solid-gas and solid-liquid systems. P.L. Richards is studying the infrared adsorption of molecules adsorbed on thin metal films using a bolometer to measure the temperature rise of the supporting substrate. This method allows one to measure the vibrational frequencies of the various molecule-substrate bonds, and is sensitive down to coverages as low as one-tenth of a monolayer. The theory groups of M.L. Cohen and S.G. Louie are supporting the experimentalists by computing the surface structure and properties of adsorbed molecules using ab initio pseudopotential calculations.

27. Why is it appropriate for DOE to fund CAM for this development? Wouldn't it be more logical to fund IBM directly if DOE wished to have this instrument developed?

It appears likely that the scanning tunneling microscope (STM) will become a tool of major importance in surface science. The device will require many years of investigation and development. It is therefore necessary for more than one group to develop this instrument in order to ensure cross-fertilization of ideas and rapid progress in the field. Furthermore development of

the STM at CAM will support other CAM research on surface science, catalysis, and electronic materials. Moreover, the presence of the instrument at CAM will make its capabilities accessible to industrial and other participants in CAM programs. In addition the STM will be available to LBL's wide-ranging program of surface science and catalysis research, and the development and utilization of the STM in this environment will lead to unique interactions among a number of investigators that should result in new and important contributions to surface science.

28. What is the "track record" of the CAM investigators in this program as to the development of advanced surface instrumentation?

Program leader, J. Clarke, has a 19-year record of very successful development of ultrasensitive instrumentation. He has pioneered the development of the modern SQUID (Superconducting Quantum Interference Device), a device for measuring extremely small magnetic fields, voltages, displacement, etc. This work has lead to the commercial realization of the device (S.H.E. Corporation). An important energy-related application of SQUIDS, namely remote-interference magnetotellurics (a technique for geophysical surveying) was also pioneered by Clarke. This technology was rapidly transferred to the commercial survey industry and is now almost universally used. This innovation was recognized by the Best Paper Award of the Society for Exploration Geophysicists in 1979, and the "Technology 100" honors list in 1980. Clarke has published about 125 papers on SQUIDS, superconductivity, tunneling, noise and geophysics.

Marvin L. Cohen, Professor of Physics, U.C. Berkeley, is a Fellow of the American Physical Society and a member of the National Academy of Sciences. He has received a Sloan Fellowship (1965 - 1967), a Guggenheim Fellowship (1978) and the Oliver E. Buckley Prize for Solid State Physics (1979). Scope of Dr. Cohen's research includes the theory of the electronic and structural properties of solids: optical, photoemissive, superconducting, vibrational, phase transitions, and surfaces; and the development of theoretical techniques in condensed matter physics with emphasis on pseudopotential theory. Recent consultations with industry include Xerox Research Labs, R&D Associates and LANL.

Paul L. Richards, Professor of Physics, U.C. Berkeley is a Fellow of the American Physical Society. He is the recipient of the Guggenheim Fellowship (1973-74), the California Scientist of the Year (1981) and the Humboldt Senior Scientist Award (1982). The scope of his research includes the development of infrared and millimeter wave detectors, the development of new techniques for infrared measurements of the vibrational spectra of molecules chemisorbed on metal surfaces, measurement of infrared properties of materials, and the measurement of spectrum of cosmic microwave background at infrared wavelengths. Recent service to government includes NASA Operations Group for Airborne Astronomy, NASA Ames Research Laboratory (Director's Review Panel), and the National Radio Astronomy Observatory Visiting Committee.

Yuen Ron Shen, Professor of Physics, U.C. Berkeley, is a member of the American Physical Society and the Optical Society of America. He is the recipient of a Sloan Fellowship (1966 - 1968), Guggenheim Fellowship (1972 - 73), Vinton-Hayes Fellowship (Harvard, 1972). Scope of his research includes

nonlinear optics, studies of condensed matter physics, surface physics and molecular physics. Recent service includes membership on the Joint Council on Quantum Electronics. Ex-Officio Member of Quantum Electronics and Applications Society and Membership of Steering Committee of 1983 International Conference on Lasers. He is the 1983 winner of outstanding Scientific Accomplishment, Solid State Physics, DOE Materials Sciences Research Competition, for "Surface Nonlinear Optics as a Novel Surface Probe."

Steven G. Louie, Associate Professor U.C. Berkeley, Recipient Sloan Foundation Fellowship (1980 - 1983), NSF Postdoctoral Fellowship, consultant to Exxon Research and Engineering. Areas of research include: Principal Condensed Matter Theory, Surface Physics, Electronic Structure Theory.

29. What other research in catalysis is DOE funding in either the BES Program, the Fossil Energy Program, or any other program? What catalysis research is being supported by other agencies, such as the NSF, or by industry?

DOE in BES is funding an appreciable number of catalysis programs. Almost all of the projects are carried out in narrow areas by individual investigators and not by interdisciplinary teams. Fossil Energy is primarily funding process development programs, not fundamental background research. NSF also supports a few programs of individual investigations similar to BES. Industry does a great deal of applied research and development but in general cannot justify the long term, high risk research in new areas of catalysis in which industrial applications may be based ten years from now.

The CAM Catalysis Program not only contains surface chemists but also synthesis chemists, theoretical physicists and experimental physicists. This unique combination is not found elsewhere. Two of the individuals (Somorjai and Heinemann) have extensive experience in consulting with industry and leading industrial research, respectively.

NSF also supports a few programs for individual investigators at select universities. The CAM program does not duplicate these existing efforts.

30. How much funding will the catalysis program receive in each of FY 1984 and FY 1985? Please include operating expenses and capital equipment.

Operating expenses are $620,000 for FY 1984 and $740,000 for FY 1985.

Capital equipment is not subdivided by program since major instruments and equipment are used on more than one program. The total equipment funding for CAM is $1,200,000 for FY 1984, $600,000 for FY 1985. A solid state Nuclear Magnetic Resonance unit and a Fourier transform I-R spectrometer are examples of instruments that will be used on more than one program.

31. Please identify specific program milestones for FY 1984, FY 1985, and FY 1986.

<u>General</u>

Broaden program by inclusion of industrial fellows and by hiring at least two LBL staff scientists with experience in synthesis or in catalysis.

Zeolites

FY 1984: Prepare and characterize two or three zeolites and study variables of synthesis conditions. Begin study of nucleation with NMR and Raman Scattering. Begin preparation of zeolites in non-aqueous media.

FY 1985: Continue synthesis with major emphasis on nucleation. Use NMR not only for characterization but also to determine effect of templates during synthesis and electron microscopy to study dispersion and location of metals in the zeolite structure. Two industrial fellows to join project.

FY 1986: Explore new routes to zeolitas synthesis. Investigate the nature of active catalytic sites by model reactions.

Transition Metal Compounds

FY 1984: Study preparation of carbides and nitrides of Group IV to VI transition metals and of silicides of Group VIII metals. Systematically vary structural, chemisorptive and catalytic properties.

FY 1985: With the help of at least one industrial fellow, begin study of mixed metal compounds or of compounds containing two non-metals, such as carbonitrides and carbosilicides. Study low temperature plasma techniques for achieving non-stochiometric compounds with unusual structures.

FY 1986: Studies of oxides, sulfides, oxysulfides, and oxycarbides of transition metals begins.

Novel Materials and Reaction Conditions in Catalysis

FY 1984: Novel organic and metallo-organic monomers will be synthesized with electronic structure tailored to give conducting polymers. The immobilization of known polymers capable of binding transition metals in electrodes will be investigated. Catalytic reaction studies of laser and plasma excited molecules will commence.

FY 1985: Novel organic and metallo-organic monomers will be subjected to polymerization using initiator chemicals, light or heat. The properties of the polymers with respect to solid state and catalytic behavior will be investigated. These systems will effect electron-transfer mediation to and from potential electrocatalysts incorporated in polymer films. Model catalytic studies will be initiated. The relationship between the excitation energy and excited state distribution of molecules and their reaction selectivity will be explored.

FY 1986: Organo-metallic molecules and enzymes will be anchored to polymer surfaces and their catalytic behavior will be investigated. The chemical behavior of laser heated and rapidly quenched catalyst surfaces will be explored.

32. How will the CAM catalysis program complement, supplement, or duplicate research being conducted at the MMRD or at other institutions such as the Center for Catalytic Science and Technology at the University of Pittsburgh, the California Institute of Technology, Eastman Kodak Company, UOP, Inc., Mobil Research and Development Company, Exxon Research and Engineering Company, and so on? How many of these performers of catalysis research were consulted in the development of the CAM program in this area?

The CAM catalysis program concentrates on research in areas other than the program mentioned in the question. Instrumental development at CAM would find application in other programs.

Twenty three organizations of the type listed in the question were represented at the workshop for the Catalysis Program, including four of the six explicitly listed. The attendees are listed in the Workshop report. The recommedations of the workshops were incorporated into the program.

The interdisciplinary, focussed, long range basic research that is the trademark of the CAM catalysis program is a very different concept of operation than the way the other programs are structured.

33. What unique physical properties of catalysts are being measured or explored that other ongoing research is not investigating? What is the uniqueness of the CAM program?

The uniqueness of the CAM approach lies in the ability to use many different tools on the same catalyst and catalytic system rather than have various individuals investigate catalysts and systems that differ in composition and operating conditions. The CAM investigations aim to establish the atomic scale properties of catalysts (structure, composition, oxidation states, etc.) and relate them to reaction parameters (rates, selectivities, lifetime, methods of synthesis and regeneration). A broad, but focussed program like this requires an interdisciplinary approach that is also unique to CAM. The interdisciplinary approach of surface science chemists, synthesis chemists, theoretical physicists and experimental physicists is, indeed novel. The industrial participation in the research is yet another unique feature.

34. What is the "track record" of the CAM investigators participating in the processing, production, and other aspects of the CAM catalysis program?

The leader of the CAM Catalysis Program, Dr. Gabor Somorjai, Professor of Chemistry of the University of California, Berkeley, is probably the world's most outstanding chemically oriented surface scientist. He is the author of over 300 scientific papers and two textbooks in the fields of Surface Chemistry, Heterogeneous Catalysis and Solid State Chemistry. He is a member of the National Academy of Sciences, a Fellow of the American Physical Society, a Guggenheim Fellow, and has been invited to give numerous distinguished lectureships both in this country and abroad. The deputy leader (Dr. Heinz Heinemann) had a long and distinguished record of catalysis research with Mobil Corporation before coming to LBL. Other investigators, although younger, are similarly of the highest quality and with accomplishments proportional to their age.

40-574 O - 85 - 63

35. The ad hoc Panel (i.e., the Narath Panel) recommended deferral of the materials synthesis laboratory and instead recommended that LBL consider strengthening the materials synthesis effort in the MMRD "consistent with CAM growth." Given these recommendations, why is CAM requesting funding for an Advanced Materials Laboratory at this early stage?

The Narath Panel recommended that construction of the AMSL/ADCL building be deferred from FY 1984 until a review of a new program plan has been completed. This has been done and the time is consistent with plans and needs.

The panel stressed the critical role of new materials in an advanced-materials program and made two important observations that LBL management has seriously considered.

1. The Panel questioned whether organizing materials synthesis in a separate, directed programmatic activity is wise and suggested that "integration of these activities into other CAM programs will be found advantageous."

The Panel's advice to integrate materials synthesis activities into a redefined CAM program was heeded. On November 3, 1983, at the third semiannual review of CAM, DOE was presented a revised CAM program plan consisting of three program areas: Electronic Materials, Structural Materials, and Surface Science and Catalysis. Materials synthesis has been integrated into each new program area. The Surface Science and Catalysis Building will house the Surface Science and Catalysis Program. Together the Electronic Materials and Structural Materials programs constitute a broad Advanced Materials program and would occupy the proposed Advanced Materials Laboratory (AML). The kind and amount of modern laboratory space needed to conduct the Advanced Materials program was presented to DOE at the November review and formed the basis for the FY 1985 request for construction funds.

2. To encourage beneficial interactions between MMRD and CAM and to maintain a balance in materials synthesis research, the Panel suggested that LBL consider strengthening the materials synthesis effort in the MMRD "consistent with CAM growth."

Though it is LBL's intention that the outstanding work in materials synthesis in MMRD will continue, it is of the "basic research push" type described by the Panel, not the "technology-pull" type suitable for CAM.

Whether LBL's materials synthesis effort is strengthened in CAM or in MMRD, the additional space and modern facilities of the AML are essential. MMRD research space is fragmented among 13 buildings, none adequate for necessary state-of-the-art synthesis facilities in electronic materials or particle processing.

DON FUQUA (Fla.), Chairman

ROBERT A. ROE, N.J.
GEORGE E. BROWN, JR., CALIF.
JAMES H. SCHEUER, N.Y.
RICHARD L. OTTINGER, N.Y.
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U.S. HOUSE OF REPRESENTATIVES
COMMITTEE ON SCIENCE AND TECHNOLOGY
SUITE 2321 RAYBURN HOUSE OFFICE BUILDING
WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Robert H. Pry
Gould, Inc.
10 Gould Center
Rolling Meadows, Illinois 60008

Dear Dr. Pry:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

QUESTIONS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

DR. PRY

1. You stated that the Materials R&D report addresses steps that might be taken to better couple DOE materials activities with industry, and that some are beginning to be implemented with surprisingly good results. Would you please elaborate?

2. What specific results of DOE's materials research have found their way to the private sector?

3. Is the current balance of DOE materials R&D among the laboratories, universities, and industry optimal? If not, which should be relatively larger or smaller?

4. Are any of the outputs of DOE materials R&D programs being incorporated into energy systems?

5. If DOE really wanted to better couple its materials R&D with industry, should it not be providing more funding for industrial performers of materials R&D?

Gould Inc.,
10 Gould Center, Rolling Meadows, Illinois 60008
Telephone (312) 640-4000

GOULD
Electronics

March 6, 1984

Chairman Don Fuqua
U.S. House of Representatives
COMMITTEE ON SCIENCE AND TECHNOLOGY
Suite 2321 Rayburn House Office Bldg.
Washington, DC 20515

Dear Chairman Fuqua:

Thank you for your letter of February 28 requesting answers to some questions concerning my testimony on February 23.

Unfortunately I did not receive your questions until it was too late to do them justice. Nonetheless I have answered them as best and as quickly as I could to get my answer back to you by March 9 as you requested.

On the subject of materials research results and their use by industry, one can make up longer lists of items than I have done here. However, the list that results, all be it impressive, is small compared to the money spent. Let me hasten to add that most industrial labs do not achieve many results until nearly ten years into a completely new program area. The only area older than ten years in the DOE labs is nuclear materials, where they have done a good job. That is why we stressed in the materials report <u>how</u> programs are chosen and <u>how</u> they are managed and <u>how</u> they are transferred to industry rather than judge detailed programs and results to date.

If I can be of any further help, please call on me.

Sincerely,

Dr. R.H. Pry

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COMMITTEE ON SCIENCE
AND TECHNOLOGY

QUESTIONS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

DR. PRY

Question 1.

You stated that the Materials R&D report addresses steps that might be taken to better couple DOE materials activities with industry, and that some are beginning to be implemented with surprisingly good results. Would you please elaborate.?

Answer:

The materials R&D report recommended that Government Laboratories and DOE be given more freedom to provide patent wavers, grant exclusive licenses, sign proprietary agreements and perform certain consulting services for industry, for money, with incentives to the laboratory people that would take such initiatives.

My knowledge is, of course, limited but I do know that the amount of interaction between Oak Ridge and Argonne with industry in the materials area has improved dramatically over the recent past. For example:

Argonne is forming an Electrochemical Industrial Associates Program for Industry. Members work cooperatively with Argonne in the area of corrosion, oxidation and electrochemical reactions of materials.

Argonne, in cooperation with the Industrial Research Institute held a conference "Spotlight on Argonne" to tell industry what Argonne was doing of interest to them. Subsequently for example, three firms led by Linbergh Co. are developing a joint program on corrosion of iron alloys and these companies are planning to put a post doctoral fellow at Argonne to assist in the program. Also, Eagle Pitcher Co. has made arrangements to get and test special glasses made by Argonne for Sodium Sulphur battery applications to determine their applicability for special batteries for Defense use.

In addition to these recent examples, Exxon Corp. had a research worker at Argonne for two years working in the area of corrosion resistant alloys. The refractories

industry also has had a joint program with Argonne for the testing and development of refractories for Coal top Gasification. These developed materials are being planned for the Cool Water plant being built by EPRI and Westinghouse.

Without detailing more specifics, I can assure you that my fellow members of the Industrial Research Institute (composed of Vice President of Research and Development of most major US manufacturing, petroleum and minerals companies) are not only more aware of our national labs but actively visit those labs and discuss programs.

Question 2.

What specific results of DOE's materials research have found their way to the private sector?

Answer:

Let me name a few examples of materials R&D results from DOE that have gotten into the private sector. These examples were not chosen for total impact as much as for diversity.

a) ONRL developed an improved 9% chromium - 17% molybdenum steel for fossil and nuclear plants. Combustion Engineering Co. is using this material for heat exchangers and piping material in steam generating equipment. It depends less on strategic materials, has better stress corrosion resistance, is tougher and has better weldability than competing steels.

b) Titanium is used widely as a replacement materials for bone in human hip joints. The life of this material can be as short as four or five years when attacked by body fluids. Oak Ridge National Labs. discovered that this life could be extended well beyond one hundred years if the titanium surface was loaded with nitrogen ions. The Zimmer Company has these new materials in for FDA approval now.

c) Lithium aluminum alloys have been shown by Argonne National Labs. to be superior to lithium calcium alloys for primary lithium batteries. These alloys are now being used in commercial lithium battery production.

d) Lastly and most important, the materials work in Nuclear materials, going back to the early work in the 1950's by Oak Ridge and Argonne, on neutron and particle irradiation of metals and alloys, to recent work on stainless steel swelling under very large neutron

irradiation doses, have been key to the US ability to build Nuclear plants with assurance of performance and is part of the required materials work for safe design of breeder and fusion plants. In addition, the work of these laboratories with the Nuclear Regulatory Commission has provided testing proceedures in existing vessels to assure continuing safety of these plants in the event of a rapid cool down after a nuclear accident.

Question 3.

Is the current balance of DOE materials R&D among the laboratories, universities, and industry optimal? If not, which should be relatively larger or smaller?

Answer:

As mentioned in the report as well as in my testimony, there is insufficient research in the area identified as Generic Materials Technology Research and Development. This specific area of research, which starts with a critical materials need in our energy systems, then picks a development approach from a combination of materials science, solid state physics or chemistry results and attempts to develop a new materials solution, including processing, composition and structure that yields the desired materials properties in a sufficiently reproductable way so as to prove technological and economic feasability.

I mentioned the recent work at Oak Ridge on Ni_2Al containing boron providing a heretofore unknown ductility for this material as the kind of materials science result useful as a starting point for generic technology development of high temperature materials for heat energies.

Similarly interesting results are being achieved from Oak Ridge and from MIT using sol gel chemistry and a variety of ultra small ceramic composition particles to form the starting point for a tough sintered ceramic heretofore unknown. This result could form the basis for a broad generic materials technology program in high temperature tough ceramics for heat engines and other applications above 1400 degrees C.

Such programs, once begun, are ideal areas for increased joint participation by user industries (engine manufacturers), producer industries (specialty metals and ceramics producers), and university and government laboratories. These groups could, in combination, make excellent accelerated progress in bringing such

materials to a usefull state; University and Government Labs broadening the science base needed to develop such materials; user Industries redefining and refining materials specification through testing of candidate materials and systems design studies; Producer Industries working out the range of compositions, structure, processing and economics required to produce the revised specified materials.

Since this area of research and development is largely missing in the DOE program, I much admit that more industry work of this kind is needed to bring the program in balance. This is very different than saying more industry work or university work is needed in the kind that is now being done.

Question 4.

Are any of the outputs of DOE materials R&D programs being incorporated into energy systems?

Answer:

Perhaps the most important stream of material results are those of nuclear materials discussed breifly under question 2 (d). Without that Government Laboratory effort I do not believe a nuclear industry would have been possible in the US and perhaps not in the world.

Again I will only site a few additional examples:

a) The low enrichment fuels program at Argonne and the development of Uranium Silicide alloys will now allow research reactors in the US and around the world to be fueled with safe low enrichment fuels. This will allow important research to continue without the risk of dispersed high enrichment fuels.

b) Argonne developed, silicon carbide, thin tube heat exchangers are now being made by The Carborundum Co. and The Norton Co. and being tested by Solar Corporation for coal gasification and then high temperature heat exchanger applications.

c) Ion implantation and subsequent laser analysis of solar cells is now in the early stages of production at Heliometrics, a California based company.

Question 5.

If DOE really wanted to better couple its materials R&D with industry, should it not be providing more funding for industrial performers of materials R&D?

Answer:

I believe this question is covered under question 3. Having industry perform more of the work that is now being done by Government and University Labs would not, in my judgement, better couple to industry. What is needed is the generic technology work in materials that was discussed under question 3.

The kind of coupling needed most, in my opinion is covered by a recent letter I wrote to Al Trivelpiece of DOE. I have attached a copy of that letter. I cannot over stress the need for our National Laboratories personnel to reach out to get information from industry on new need oriented programs and then to go out and promote their solutions to industry.

C-O-P-Y

February 2, 1983

Dr. Alvin W. Trivelpiece
Director, Office of Energy Research
Department of Energy
Washington, D.C. 20585

Dear Al,

Thank you for your recent letter on the subject of technology transfer. I apologize for not meeting your deadline of February 1, but the planning and execution of a general reorganization of Gould has kept me somewhat occupied recently.

Technology transfer, to me, has always implied an outreach program, an evangelistic effort, and crusade. As I'm sure you are well aware, there is no tougher thing in the world to sell than an idea. It is relatively easy to explain an idea to others and to have them understand what you have explained. For technology transfer this is not enough. By technology transfer we imply that what is transfered is the enthusiasm for the idea and the dedication to make the idea useful to the society.

To use an analogy, when a preacher preaches on Sundays, he does not necessarily transfer religion or religious beliefs, although most of the congregation that remain awake would be able to understand and repeat the substance of what he says. The transfer here implies that the person preached to actually changes his behavior in the desired manner as a result of the sermon. If you believe this transfer is a simple task, I suggest talking to even a successful preacher for an update on his success ratio.

The concept of techology transfer; i.e. its success being measured by the action of the receiver implies that the process is a very personal one. It follows then that technology transfer is most easily accomplished by transfering the person who has the technology, the faith in its importance and the ability to realize its application potential into an organization willing to support the exploitation of the technology.

If this is not possible, then technology transfer, just as any other successful sales campaign requires:

1) The choice of a person or persons responsible for "selling" the idea with a reward system for success.

2) The Identification of a list of "prospects" to utilize the idea.

3) An outreach program to potential receivers or customers to understand the possible barriers to the sale or transfer.

4) An effort to either overcome the barriers to acceptance or to alter the technology or idea to be transfered to go around any barriers that legitimately exist.

5) Get the prospective recipients involved so they can claim some "authorship" in the transfered idea for themselves.

6) Once the recipient is "on the hook" and attempting to exploit the technology then providing a sufficient overlap of time for help and reinforcement (a warranty period in sales terms) to make sure that follow through to the market place actually occurs.

It may be that the government organization is not prepared to undertake all of these steps. If it is not, it must nonetheless recognize that these steps must be taken by someone. The originating government organization must somehow see to it that someone becomes the successful broker.

Rather than go into too much detail, a little reflection will suggest what has and has not been done successfully in various programs. In my discussions with lab personnel and with universities, there is a popular conception that a technology transfer program means removing positive internal barriers to outside people coming in and getting information. I try to tell people with this belief that this approach is like my lead salesman saying that he is sure that our sales will now go up because, although he is still not making sales calls, he has opened his door and installed a telephone!

What specifically might be done to enhance technology transfer from DOE?

1) Experiment by asking a research scientist or engineer from each division in the GOCO labs to take a two year reversible assignment to connect his division work to selected external companies. (Make sure he has the travel budget to do the job)

2) Provide internal incentives and awards for laboratory people whose ideas have been picked up by industry.

3) Increase the number of open house activities. Advertise and structure them around items developed at the lab that my have industry value (e.g. measuring and control instruments, motors and servos, application software, materials, and processes).

4) Encourage internal instrument development and maintenance type activities to set up shop "outside the fence" as independent contractors to create well coupled technical entrepreneurs that will take lab developments to external markets.

5) Start a program of one year sabbaticals between industry and the GOCO labs in both directions.

As you can see, the kind of suggestions I am making are almost all people centered. I can't emphasize this approach enough.

Hope this is of some help.

Sincerely,

Robert H. Pry,
Vice Chairman
Technology

RHP/a

DON FUQUA (Fla.), Chairman

GEORGE E. BROWN, JR., CALIF.
JAMES H. SCHEUER, N.Y.
RICHARD L. OTTINGER, N.Y.
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COMMITTEE ON SCIENCE AND TECHNOLOGY
SUITE 2321 RAYBURN HOUSE OFFICE BUILDING
WASHINGTON, D.C. 20515
(202) 225-6371

February 28, 1984

Dr. Frederick Seitz
Rockefeller University
1230 York Avenue
New York, New York 10021

Dear Dr. Seitz:

Thank you for your excellent testimony before the Subcommittee on Energy Development and Applications on February 23, 1984. Attached are some additional questions that Members of the Subcommittee would like you to answer, in order to supplement the record of the hearing on this topic.

I would appreciate your responses to these questions by March 9, 1984. If you have any questions regarding this request, please contact Dr. Harlan Watson of the EDA Subcommittee staff at (202) 225-4320.

Sincerely,

DON FUQUA
Chairman

DF:Hcw
attachment

QUESTIONS

FY 1985 DOE Authorization for
Supporting Research and Technical Analysis

February 23, 1984

DR. SEITZ

1. You stated in your testimony that you expect the Committee's interim report to be completed by mid-June 1984. When do you expect the final report to be completed?

2. In light of the recent studies of materials sciences and major facilities we have heard about today, what new issues is your Committee's report likely to illuminate?

3. Do you see this study as satisfying the need for peer review of major new facilities in materials sciences, or is this just a first step?

4. To what extent will facility costs, including construction costs and lifetime operating and maintenance costs, be considered?

5. Will your Committee be assessing the appropriate balance of "bench-top" materials sciences research and major materials research facilities?

THE ROCKEFELLER UNIVERSITY
1230 YORK AVENUE • NEW YORK, NEW YORK 10021-6399

March 9, 1984

Dr. Harlan Watson
Subcommittee on Energy Development
Applications
B-374 Rayburn House Office Building
Washington, D.C. 20515

Dear Dr. Watson:

The responses to your five questions are as follows.

1. We expect to have a usable draft of the report available at some time in June 1984 in order to provide the sponsors of the studies and others in government with the principle conclusions of the study. The very final edited version may take several weeks longer before it is made completely public.

2. It is our hope that the work of the Committee will throw some new light on issues related to neutron sources and light sources that will serve to extend and amplify previous studies dealing with these topics. We also have a special subpanel that has the goal of looking into possible needs for large equipment of different types so that we have a more comprehensive understanding of the needs that are apt to emerge in the near future for a large equipment that would be used in the materials sciences. In this way we hope to have a better overall picture of the requirements in this field in the period ahead. In the course of the study we will pay particular attention to comments and advice received from leading individuals who are not normally users of large equipment but who are concerned that expenditures for very large equipment will curtail small scale research which has great importance in its own right.

3. In the case of equipment of intermediate size, say that costing between ten and one hundred million dollars where there have been many peer reviews to date, peer review beyond that carried out by our Committee may be unnecessary. However, our recommendations concerning much larger equipment say that in the range of two hundred million dollars or more may well require further peer review at a later date after special studies of feasibility of various forms of instrumentation to be used in connection with such facilities have been carried out.

4. It is our hope that we will be able to provide the government with reasonably fair estimates of cost of equipment in the range between say five and ten and one hundred million dollars. Cost estimates for larger equipment will inevitably be somewhat provisional and need refinement at a later date.

5. As stated above, our Committee is keenly conscious of the fact that many of the best advances in materials science are made by individuals who work at a relatively small scale. We expect to keep the requirements of such individuals well in mind, particularly when we provide recommendations for the phasing in over the coming decade or two of larger equipment.

I hope these responses will be of interest to you and your committee.

Sincerely,

F. Seitz

Frederick Seitz

40-574 O - 85 - 64

APPENDIX II

ADDITIONAL MATERIALS FOR THE RECORD

A. Narath
Executive Vice President

Sandia National Laboratories
Albuquerque, New Mexico 87185

August 31, 1983

Dr. A. W. Trivelpiece, Director
Office of Energy Research
U. S. Department of Energy
Washington, DC 20545

Dear Al:

I am pleased to transmit to you the final report of the ad hoc NCAM Review Panel. The report reflects the unanimous view of the Panel; there are no significant minority opinions. Please let me know if further elaboration on any of the findings would be useful to you.

Best regards,

Enc.

Report of the ad hoc Panel to Review the Lawrence Berkeley Laboratory Proposal for a National Center for Advanced Materials (NCAM)

A. Narath, Chairman
D. R. Davies
J. M. Deutch
J. L. Doyle
F. R. Gamble, Jr.
K. L. Kliewer
J. A. Krumhansl
D. W. Lynch
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August 31, 1983

EXECUTIVE SUMMARY

This report describes the results of a technical and programmatic review of the Lawrence Berkeley Laboratory (LBL) proposal for a National Center for Advanced Materials (NCAM). Among its several important objectives, this DOE materials research initiative is intended to establish new modes of enhanced interaction with U.S. industry. In support of the initiative the proposal calls for construction of an advanced synchrotron-radiation light source (ALS) and two major laboratory buildings at LBL, as well as several additions (SEFF) to the existing Stanford University Synchrotron Radiation Laboratory (SSRL). The review was conducted by an ad hoc Panel appointed by Dr. A. W. Trivelpiece, Director, Office of Energy Research, DOE.

The Panel adopted a set of criteria to guide its review, which are consistent, in general terms, with recommendations of recent DOE Laboratory studies conducted by the DOE Energy Research Advisory Board and the White House Science Council. These criteria are:

(1) Relevance to an advanced-materials theme.
(2) Realistic potential for significant impact on important U.S. industries.
(3) Program goals and objectives whose attainment requires centralization of research efforts.
(4) Contribution to a new or strengthened mission for LBL.
(5) Resource requirements not excessive in relation to value of projected accomplishments.

The Panel finds that although the NCAM proposal considered in detail does not adequately satisfy the review criteria, it, nevertheless, offers exciting opportunities for significant

advances in this technologically important field. Realization of the opportunities will, however, require substantial alterations of the proposal to assure

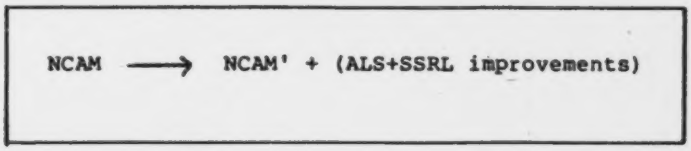
(1) a structured "technology-pull" orientation, which complements existing "basic-research-push" programs at Berkeley;

(2) selection of a limited set of topical areas of industrial importance;

(3) a directed-research approach, which encourages individual innovation while pointing the collective effort toward clearly-defined goals;

(4) implementation of close contacts with industry.

The most serious deficiency in the proposal is the combination of materials R&D and the ALS in a single initiative. Judged in terms of its potential contribution to a goal-oriented, "technology-pull" materials theme, the ALS requires a disproportionately large share of NCAM resources. It is therefore an inappropriate centerpiece which causes an unacceptable program imbalance. The Panel concludes that the two NCAM components should be decoupled and each considered on its own merits, i.e.



The materials component NCAM' is the essential part of the LBL initiative, and should be characterized by a technology focus.

The Panel believes that several actions should be taken expeditiously to assure that the NCAM' materials initiative is pointed in the proper direction from the beginning.

(1) Restate the goals and objectives to clarify the intended technology focus and ALS decoupling.

(2) Appoint an NCAM' Director who has experience managing directed-research activities and understands the needs of the industrial community.

(3) Establish an NCAM' advisory board for policy guidance, with strong industrial representation.

(4) Develop an NCAM' program plan which emphasizes major roles in a few technologically important areas of materials science.

(5) Establish an organizational structure consistent with NCAM' program objectives.

(6) Implement effective mechanisms for industrial involvement.

(7) Develop a funding strategy which integrates DOE Basic-Energy-Sciences funding with support from DOE's programmatic organizations, as well as from industry.

(8) Develop a staffing strategy which is largely independent of future availability of UC-Berkeley joint faculty appointments.

Among the three broad materials areas described in LBL's NCAM Scientific Program Summary, the Surface Science and Catalysis activity is judged to be the strongest, primarily on the basis of the quality and breadth of LBL's on-going catalysis research. The Panel strongly endorses construction of the Surface Science and Catalysis facility (SSCL) beginning in FY-84. In regard to the other two areas, Advanced Materials Synthesis and Advanced Device Concepts, final judgment of these activities should be delayed until an acceptable NCAM' program plan is available for review. Construction of the associated AMSL/ADCL facility should be deferred until that time.

While the Panel favors continued support for R&D on advanced light sources at LBL, the decision whether or not to proceed with actual construction of an ALS should await completion of a review by the synchrotron-radiation community. In the meantime, the proposed upgrade of the SSRL facility is strongly supported by the Panel, because

(1) SSRL has established an extensive user community and can point to significant scientific accomplishments,

(2) the existing SSRL support facilities are marginal in relation to existing needs and opportunities,

(3) available beam time at SSRL is inadequate to meet user demands,

(4) a hard x-ray beam line of superior characteristics can be installed on PEP at relatively modest cost.

The FY-84 funding to support the Panel's findings totals $22.5M (13.4M for construction and $9.1M for operating and equipment). The construction funds would provide $9.3M for LBL's Surface Science and Catalysis Laboratory and $4.1M for the SSRL upgrade. The recommended SSRL construction funds include $0.3M for the 18° beam-line project which the original NCAM proposal had included in the ALS line item. The operating/equipment funds would support continued development of synchrotron-radiation technology, provide modest initial growth for the surface-science/catalysis program, and provide a total of $2.0M for NCAM' program planning and "seed money" to initiate necessary staff hiring.

The FY-85 funding requirements include construction funds to assure rapid completion of the SSCL and SSRL/SEPFF projects. The Panel also supports the $12.7M request for operating and equipment detailed in the NCAM proposal. However, whether commitment of design funds for the AMSL/ADCL facility will be justified cannot be determined by the Panel at this time.

Decisions concerning FY-85 construction funding for the ALS should, of course, be based on the outcome of the independent review.

As the Panel was finishing its deliberations it learned that the FY-84 Energy and Water Development appropriation bill, while including the requested operating and equipment funds, contained only $3.0M for NCAM construction. The Panel fears that this action may force undesirable delays during the crucial formative stages of the NCAM' initiate, thereby reducing the probability of it ever being implemented successfully. For this reason the Panel hopes that it will be possible to increase the FY-84 construction funding to permit, at a minimum, start of construction of the SSCL and support of the 18° beam-line project at SSRL.

I) Introduction

This report documents the findings and conclusions of an *ad hoc* Panel which was appointed by the Department of Energy (DOE) in late March 1983 to conduct a technical and programmatic review of the Lawrence Berkeley Laboratory (LBL) proposal for a National Center for Advanced Materials (NCAM).

The proposed materials center is a major new DOE initiative in materials science. It has been presented as an exciting prospect for a new level of interaction among academic, federal, and industrial scientists. First described in the LBL FY-83 Institutional Plan, it proposes to provide a national focus for research on the synthesis, characterization, and behavior of advanced materials of importance to energy-related and high-technology industries, together with device developments exploiting materials advances. In support of this initiative, the proposal calls for construction of an advanced light source (ALS, a "next-generation" synchrotron radiation source optimized for the VUV spectral region) and two major laboratory buildings at LBL, as well as several additions to the existing Stanford University Synchrotron Radiation Laboratory (SSRL). Initial major funding was included in the FY-84 President's budget request for DOE. Funding requirements through FY-89 were estimated to be $138.9M for construction and $127.0M for R&D operating and equipment. The total of $265.9M includes $14.4M for the SSRL improvements.

The specific tasks to be addressed by the Panel were defined by Dr. Alvin W. Trivelpiece, Director, Office of Energy Research (ER), in his formal charge of March 31, 1983 (Appendix I). He requested an examination of all the elements and activities proposed for the Center including a review of the proposed facilities, organizational arrangements, and other

related matters. A revisitation of DOE's decision to establish NCAM , however, was explicitly excluded by the charge. During the Panel's initial executive session, Dr. Trivelpiece elaborated on the Panel's charge. Referring to the Energy Research Advisory Board's (ERAB) Multiprogram Laboratory Panel recommendations, he amplified his earlier statements by stressing DOE's commitment to directing Laboratory efforts into more productive areas, especially in regard to their interactions with industry. The NCAM initiative was intended to be responsive to this commitment and to serve as a guide for future redirections at other Laboratories. To assure success, Dr. Trivelpiece considered it important to explore all strengths and weaknesses of the NCAM project while improvements could still be incorporated in LBL's planning. With this clarification the Panel constrained its deliberations on only two points: (1) The choice of materials science as the topic of a new DOE National Laboratory initiative, and (2) the selection of LBL as the location for the initiative.

The report is organized as follows: Section II discusses the review methodology and lists the principal sources of information. Section III provides relevant background information. Section IV develops the criteria which the Panel adopted for its review. Section V contains the Panel's principal findings and conclusions. Section VI offers concluding remarks and a recommended NCAM funding profile.

II) Review Methodology and Information Sources

The Panel met as a group three times. The initial meeting took place April 22-23, 1983, at LBL for detailed briefings by LBL staff on the NCAM proposal, tours of existing facilities, and discussions with Dr. D. A. Shirley, Director, LBL. The second meeting was held in Washington, DC, June 6-7 for discussions with selected members of the scientific community to clarify the nature of the criticisms which the proposal had attracted. (Dr. M. Blume - Brookhaven; Prof. M. Dresselhaus - MIT; Prof. T. H. Geballe - Stanford; Dr. L. C. Hebel - Xerox, Palo Alto; Prof.C. P. Slichter - U. of Illinois). At that meeting, the Panel also held discussions with Dr. W. D. Carey - AAAS, a member of the ERAB Laboratory Panel, to gain a better understanding of that Panel's recommendations as contained in its final report submitted in September, 1982, and with Dr. R. H. Kropschot, Associate Director DOE/ER, Office of Basic Energy Sciences (BES). Following the Washington meeting, an interim summary of principal findings and recommendations was submitted to Dr. Trivelpiece at his request because of Congressional interest (Appendix II). The third meeting was held in Denver, CO, July 14-15 to formulate a draft of the final report. On the second day of that meeting the Panel was joined by Dr. R. H. Pry, Chairman of the current ERAB Materials R&D Study Panel. This interaction afforded an opportunity to compare the conclusions of the NCAM Panel with the interim findings of the much broader ERAB study.

In addition to its formal meetings the Panel benefited from extensive informal interactions between individual members and the industrial as well as academic materials science communities.

The primary source of information for this review was the material provided by LBL during the Panel's first meeting, most notably the NCAM Scientific Program Summary (LBL document PUB-5087).

Other sources of valuable information included:

(1) Records of Congressional testimony related to the FY-84 NCAM initiative;

(2) The approximately 80 letters regarding the NCAM proposal addressed to the Honorable Don Fuqua, Chairman of the Committee on Science and Technology of the U. S. House of Representatives (HST); as well as related correspondence to which the Panel had access.

(3) Proceedings and other records of the ALS/SSRL Users Workshop (5/9-11/1983), the NCAM Industrial Participation Workshop (5/23/1983), and the DOE construction review of NCAM, 4/5-6/1983, all held at LBL.

(4) LBL Materials and Molecular Research Division (MMRD) Annual Report, 1982.

(5) a number of publications broadly relevant to this review, including

- Final Report of the Multiprogram Laboratory Panel, ERAB (1982).
- LBL Institutional Plan, FY 1983-1988.
- Federal R&D and Industrial Policy, G. A. Keyworth, Science 220, 1122-1125 (1983).
- Current Status of Facilities Dedicated to the Production of Synchrotron Radiation, D. W. Lynch, et al, National Academy Press, 1983.
- Report of the Research Briefing Panel on Materials Science, T. H. Geballe, et al., National Academy Press, 1983.

- Materials Science and Engineering: Its Evolution, Practice, and Prospects, M. Kranzberg, C. S. Smith, R. S. Claassen, and A. G. Chynoweth, Mater. Sci. Eng., 37, 1-102 (1979).
- Research Opportunities in New Energy-Related Materials, J. L. Warren and T. H. Geballe, Mater. Sci. Eng. 50, 149-198 (1981).

III) Background

(A) The NCAM Proposal

It appears to the Panel that the Administration's encouragement and support of the NCAM initiative has been based in large part on two general considerations. First, there is the realization that the unquestioned lead in technology and its applications enjoyed by the U.S. since World War II has narrowed or vanished in several important fields as a result of international competition. One of the responses to this threatening trend has been to seek more effective interactions between federally-funded and industrial research activities, with the goal of enhancing the industrial R&D process. Second, there is a belief that the federal laboratories, an important national science and engineering resource, need, in many cases, to refocus their efforts on problems of greater current importance. Because of the increasing dependence of modern technology on materials, the NCAM proposal was judged relevant by DOE to both considerations.

The origin and motivation for LBL's proposal of a major materials initiative derived primarily from institutional considerations which were presented to the Panel by Dr. Shirley as follows:

(1) Concern over significant Laboratory budget reductions since FY-81 resulting largely from declining support for LBL's energy technology activities.

(2) Concern over steady erosion in LBL's high-energy and nuclear physics programs. These areas represent traditional strengths of LBL and were the primary reason for establishing LBL in 1931. In recent years primacy in these programs has either been diluted or shifted to other institutions, raising questions about LBL's future role.

(3) The existence at LBL of a large, and highly competent accelerator engineering and science staff and supporting facilities. Serious concerns have been raised for some time regarding future needs at LBL for this capability.

(4) The existence at LBL of a broad-based, vigorous MMRD (Materials and Molecular Research Division) program in Materials Science, and related topics. LBL's management has concluded that this large activity offers a promising opportunity for Laboratory redirection.

To what extent these institutional considerations relate to national needs in materials science and technology is a logically relevant question which the Panel has considered in the context of the NCAM proposal.

The Materials Center proposed by LBL features a VUV/soft x-ray synchrotron radiation source (ALS) of superior characteristics (in terms of brilliance and time structure) as the centerpiece of an expanded LBL materials R&D effort with emphasis on increased industrial participation. In addition to the ALS, the proposal involves several other major construction line items which are described in the Scientific Program Summary and are listed here for reference purposes.

(1) SSCL - Surface Science and Catalysis Laboratory

(2) AMSL - Advanced Materials Synthesis Laboratory

(3) ADCL - Advanced Device Concepts Laboratory

Functions (2) and (3) would be combined in a single laboratory building. In addition, as mentioned earlier, the NCAM proposal includes funding for SSRL improvements, namely

(4) SEPF - Stanford Extended Photon Flux Facility

The proposed funding schedule for NCAM is exhibited in Appendix III.

(B) Materials Research at LBL

The success of any research initiative, especially one with goals as ambitious as those of NCAM, depends in large measure on institutional factors. Among these, the existing technical strengths and traditions are of particular importance. In order to familiarize itself with the LBL institutional setting as it relates to NCAM, the Panel examined the history and current status of the LBL materials program. This program represents a major emphasis in LBL's Materials and Molecular Research Division (MMRD). [Although the choice of LBL as the site for a new materials initiative was not an issue to be addressed by the Panel, it was judged important to understand the existing situation before attempting to evaluate future plans.] The Panel's understanding of the MMRD history is summarized in Appendix IV.

The general character of LBL's materials program is strongly influenced by its historical roots. For example, its permanent professional staff is dominated by UC faculty, with 53 of the 63 investigator positions currently involving joint LBL/UC appointments. In addition, the program now includes 361 graduate students and 142 postdoctoral and other visiting scientists. Because of the stringent faculty screening process, the MMRD staff represents an unusually talented and productive group of investigators. Not surprisingly, the program consists of a large number of essentially uncoordinated, small scale investigations covering a very wide range of subjects, not unlike typical university programs. The broad scope of the research is illustrated by the Table of Contents (reproduced in Appendix V) of the 1982 MMRD Annual Report.

(C) Summary of Community Responses

An extensive body of information existed prior to the present review, much of it in correspondence to the Honorable Don Fuqua, Chairman, HST, documenting the initial reactions to the NCAM initiative from the scientific community. Broadly speaking the comments divide into two classes, depending on the institutional affiliation of the correspondent.

The industrial reactions covered a broad spectrum of views. On balance these responses endorsed the concept of an LBL materials initiative emphasizing creation of closer Laboratory/industry ties. Though supportive in principle, a variety of specific concerns were raised centering on perceived inconsistencies between stated NCAM objectives and the proposed implementation of the program.

The university responses were distinctly different; most of these were unequivocally negative. The criticisms concentrated predominantly on the lack of adequate peer review for an initiative whose essence was perceived to be academically oriented. (This reaction is understandable in view of the historically strong dependence of LBL's materials research on UC faculty staffing.) Another common criticism concerned the centralized approach to materials research inherent in NCAM; it is a widely held belief in academic circles that greater progress could be achieved by dispersing the incremental funding among existing institutions on a competitive basis. The initiative was also seen as a threat to continued funding of established programs because of the large NCAM resource requirements in relation to the present size of the national university-based materials research enterprise. Despite DOE assurances that NCAM funding would not come at the expense of existing materials programs, concerns over adverse

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future budget impacts have persisted. Anticipation of seriously disruptive losses of senior staff to NCAM has further intensified these concerns.

Much of the NCAM controversy focusses on the ALS. The following sampling of questions captures the essential content of the debate:

(1) How vital are more synchrotron radiation sources to advanced materials, in comparison with other research tools competing for scarce resources?

(2) Does the VUV/soft x-ray region offer the best opportunity for the next major capital investment? Is the hard x-ray region more important?

(3) Will radiation sources currently operational or under active development really be oversubscribed by the end of the decade?

(4) In view of continuing rapid advances in synchrotron radiation technology, is it wise to commit <u>now</u> to a specific design?

(5) Assuming a next-generation synchrotron radiation source is justified, is LBL the best location? Would expansion at an existing site be less costly?

(6) Given the existing state of synchrotron radiation technology, are the superior ALS specifications technically achievable with reasonable confidence on the proposed schedule?

Other important issues raised involved the scope of materials-science topics, their technological relevance, modes of management direction and mechanisms for industrial involvement.

IV) Review Criteria

Very early in its deliberations the Panel realized that the absence of a consensus supportive of NCAM stemmed from conflicting agendas. Viewed from the perspective of LBL's capabilities, traditions and current institutional concerns, the NCAM proposal is easily understood. However, viewed from a broader national perspective serious problems emerge. In order to assure the desired balanced point of view, the Panel adopted several review criteria which, while retaining sensitivity to local considerations, were tied strongly to national perspectives.

As a starting point, the Panel kept sight of the following DOE objectives:

(1) To treat the National Laboratories as institutions rather than sites where unrelated technical work is performed and to seek new missions where necessary to assure their continued vitality.

(2) To redirect, where necessary, Laboratory efforts into areas of greater relevance to national needs, both scientifically and technologically.

(3) To define new modes of enhanced interaction among the Laboratories, industry and universities.

The task of developing acceptable criteria was complicated by the recognition that DOE materials R&D, unlike high-energy physics, does not readily qualify for a "national trust" designation and must therefore be viewed in a mission-support context. At the same time, the Panel believes that an urgent need exists in the U.S. to accelerate the translation of basic knowledge into new technology. A more rapid and efficient transition between results of basic research and industrial applications remains a major challenge for the scientific community. More effective coupling

mechanisms between research and development, as well as practical approaches to improved selectivity in the pursuit of new knowledge are among the important issues which have generated considerable discussion. The Panel notes that the prospects for achieving significant near-term gains are especially encouraging for materials science. First of all, it is a subject of great industrial importance because of the essential and often limiting role of materials in modern technology. Moreover, advances in the state of knowledge in supporting scientific disciplines such as condensed-matter physics and chemistry, as well as relevant engineering disciplines, offer growing opportunities for the development and utilization of advanced materials. Underlying its subsequent conclusions, the Panel made the reasonable assumption that a materials research program directly aimed at contributing to the crucial knowledge-to-application transition can form the basis for a DOE mission assignment. (The required overlap between the chosen materials topics and DOE programmatic responsibilities is a policy matter which will require additional examination.)

The Panel also recognizes that the materials field is extremely broad and diverse. Any individual program or laboratory focus can at best address only a small segment of the subject, making thoughtful selection of topics an essential requirement.

Guided by these considerations, the Panel decided to evaluate the NCAM proposal according to criteria which can be represented qualitatively by the following set of desired attributes:

(1) Relevance to an advanced-materials theme
(2) Realistic potential for significant impact on important U.S. industries, consistent with

established policies regarding federal laboratory/industry interactions and DOE responsibilities.

(3) Program goals and objectives whose attainment requires centralization of research effort.

(4) Contribution to a new or strengthened mission for LBL, justifying the claim of a laboratory redirection.

(5) Resource requirements not excessive in relation to value of projected accomplishments.

These criteria are consistent, as the Panel understands, with the recent report of the Federal Laboratory Review Panel of the White House Science Council (The Packard Panel).

V) Findings

(A) General Observations

It is the opinion of the Panel that the NCAM proposal, considered in detail, does not adequately satisfy the criteria developed above. Nevertheless, the Panel concludes that the establishment of a materials center at LBL offers exciting opportunities for significant advances in this technologically important field. Realization of these opportunities will, however, require substantial alterations of the proposal to assure that:

(1) a structured "technology-pull" orientation is achieved which complements the more traditional unstructured "basic-research-push" orientation of LBL's MMRD.

(2) careful selection of a limited set of topical areas is accomplished, which build on existing MMRD and/or university strengths at Berkeley and are of demonstrable interest and importance to the concerned segments of the industrial community.

(3) the research is tightly structured, and directed in such a way as to encourage individual innovation while maximizing constructive interactions among the various activities. At the same time the collective effort should be pointed toward clearly-defined and understood goals and objectives. It is this combination of features which distinguishes those large-scale materials research efforts, e.g., Bell Laboratories, which have consistently achieved significant impacts on technology. Realizing such collective effects demands a centralized organizational arrangement as envisioned for NCAM.

(4) procedures are implemented to maintain close contacts with industry in regard to program definition, priorities, execution, and termination as appropriate.

The importance of a technology focus cannot be over-emphasized. It would, of course, be a far easier task for LBL's management to treat the NCAM initiative as an extension of current materials activities, not differing substantially in character from the wide-ranging, loosely-structured approach of the MMRD, or, for that matter, of the NSF-supported Materials Research Laboratories. To be sure, such an arrangement would provide a significant stimulus for LBL. Laboratory revitalization by budget augmentation alone, however, is inconsistent with the ERAB and White House Science Council recommendations. Such an approach would also present little justification for bypassing the traditional peer-review process for academically-oriented research, and for concentrating a large increment of materials-science support at a single institution (especially one whose university ties are as intimate as those at LBL). Consequently, this approach is likely to exacerbate NCAM-related tensions between DOE and large segments of the scientific community. In this connection it is worth noting that the Panel regards a technology focus as the most persuasive justification for continuing the NCAM funding as an increment in future DOE budgets. Finally, a "more of the same" implementation of NCAM would constitute rejection of an important opportunity to direct a sizable fraction of LBL's program toward greater technological relevance, and to create thereby a real mission context for its materials activities.

Returning to the matter of deficiencies in the NCAM proposal, the Panel finds that the proposal exhibits a major flaw by combining two weakly related and mutually interfering components in a single package -- namely materials R&D and the ALS. The Panel fully recognizes that synchrotron radiation has become an important research tool in materials science, as it has in other fields. Nevertheless, judged in terms of its

potential contribution to a goal-oriented, "technology-pull" materials theme, the ALS requires a disproportionately large share of NCAM resources. It is therefore an inappropriate centerpiece which causes an unacceptable program imbalance. The materials component suffers loss of credibility because the ALS is a heavy burden which would inevitably divert NCAM resources and management attention. In fact, it is likely that the materials program would in time become captive in substantial measure to technical challenges facing development and operation of the ALS, instead of the ALS supporting the materials initiative, as proposed. Failure to establish the recommended industrially-motivated technology focus is therefore almost assured at the outset.

The ALS also suffers because a compelling justification based on materials relevance alone cannot be constructed at this time. Unfortunately, as a result of its identification with the NCAM initiative, only limited incentive has been provided so far for exploring the utility of the unique features of the ALS in other fields, especially biology.

By this line of reasoning the Panel is led to the conclusion that the two principal components of NCAM should be decoupled and each considered on its own merits. In other words

$$\text{NCAM} \longrightarrow \text{NCAM}' + (\text{ALS} + \text{SSRL improvements})$$

with the materials component NCAM' being characterized by a technology focus as discussed above, and the ALS (and SSRL) by a user-facility focus in the usual sense. It also appears advisable to rename the materials component to be more

consistent with the true nature of the initiative; e.g., NCAM' ⟶ BCAM (Berkeley Center for Advanced Materials).

If (or when) a convincing justification for an ALS is established, a strong case for locating such a facility at LBL can be made, despite the NCAM decoupling, as will be discussed briefly later in this report.

(B) Materials Initiative (NCAM')

Overall, the proposed materials program lacks strategic content, as illustrated by the following observations:

(1) In its present proposal form the program, with few exceptions, comprises an extensive compilation of potentially interesting topics. As a consequence, it is far too broad in scope and lacks coherence and focus. The plan, if followed, would encourage too many unrelated directions for the proposed funding level, even if the incremental R&D funding reaches $28.5M by FY-89 as proposed.

(2) It does not appear that an adequate effort has been made to relate the proposed work to current research either in industry or other universities and federal laboratories.

(3) The heavy emphasis on justifying the ALS in the context of materials R&D distorts the presentation considerably.

(4) The enhanced modes of interaction with industry are not developed adequately. Similarly, the technology focus does not emerge convincingly from the discussion.

(5) The future relationship between NCAM' and the MMRD is not addressed in sufficient detail.

(6) The proposed organizational structure based on facilities is far from optimum. This problem is illustrated by the awkward separation of materials synthesis from other program elements.

(7) The proposed program lacks adequate chemical integration. Materials Science is an interdisciplinary subject and chemistry is one of its vital contributors.

The materials program described in LBL's Scientific Program Summary is organized around the three laboratories, SSCL (Surface Science and Catalysis), AMSL (Advanced Materials Synthesis), and ADCL (Advanced Device Concepts). Among the three areas, the Surface Science and Catalysis activity is judged by the Panel to be the strongest, primarily on the basis of the quality and breadth of LBL's on-going catalysis research. The Panel also regards this area as technologically extremely important and promising, and therefore an appropriate choice for increased support. For these reasons, the Panel strongly endorses construction of the SSCL facility beginning in FY-84. This laboratory was authorized several years ago. It is regrettable that no funds have been appropriated to date for its construction. Although the Panel is convinced that an expanded effort in the Surface Science and catalysis area at LBL is fully justified, it remains for LBL to complete a coherent plan which is in harmony with NCAM' objectives.

It is instructive to consider the catalysis program as an example of the general approach to NCAM' implementation favored by the Panel. As proposed, the program is limited to zeolites and draws on only a small fraction of the rather formidable array of relevant talent available at Berkeley. As NCAM' is more fully developed, the Panel would like to see features such as the following appear in the plan:

(1) The formation of one or more catalysis research working groups with representation from appropriate industries, as well as university and National Laboratory groups. These working groups, with

guidance from LBL management, would plan and execute specific program elements at LBL and participating institutions, as appropriate.

(2) An explicit, thorough analysis of the long-range U.S. needs in the field of heterogeneous catalysis, based on a consideration of likely future scenarios with regard to the price of oil and/or strategic metals.

(3) An analysis of the current industrial, university and federal laboratory catalysis efforts so as to position the NCAM' program to complement rather than duplicate them.

(4) The identification of outstanding current problems in catalysis which are beyond the means or charter of U.S. industrial laboratories.

(5) Development of research programs to create better tools for the evaluation and characterization of practical catalytic systems in realistic environments.

(6) A substantial synthetic chemistry effort to create in a systematic fashion new classes of materials of catalytic significance in which trends in catalytic activity can be studied along with variations in other properties, both electronic as well as structural.

(7) A more integrated effort overall, i.e., one that incorporates all the relevant disciplines:e.g., condensed-matter physics, chemistry, surface science, and chemical engineering. These are all disciplines in which Berkeley excels.

What would be the results of a successful catalysis effort? Several can be mentioned, for example, the

generation of a more complete relevant science base to support the nation's industrial efforts; the discovery of catalytic approaches to some of the nation's more distant needs such as those associated with synthetic fuels and coal-derived industrial chemicals; possibly, in conjunction with industrial teams, the development of commercially useful catalysts where the skills and facilities of NCAM' provide unique resources necessary for such advances.

The catalysis area is one in which industrial participation may be especially difficult to achieve because of the sensitivity of most U.S. industrial concerns to catalysis-related proprietary rights and trade secrets. If mechanisms for effective cooperative efforts are found in this area they should be easily adaptable to other NCAM' programs. In this regard it is noteworthy that several of the LBL scientists have extensive experience in major industrial laboratories active in catalysis.

In regard to the two other areas, Advanced Materials Synthesis and Advanced Device Concepts, the Panel believes that final judgment of these activities should be delayed until an acceptable NCAM' program plan is available. Construction of the AMSL/ADCL facility should therefore be deferred until a subsequent review of that plan has been completed.

The Panel questions whether organizing materials synthesis as a separate, programmatic activity is wise. The same concern applies to the device activity. It seems likely that integration of these activities into other NCAM' programs will be found advantageous. However, the Panel also recognizes that innovative research in chemical synthesis and related activities (i.e., the creation and subsequent characterization of novel, potentially useful materials) is not always most

productive under the pressures of a directed program. Because of the critical role of new materials in an advanced-materials program, it is highly desirable that balance be maintained in materials-synthesis research. For this reason the Panel suggests that LBL consider strengthening the materials-synthesis effort in the MMRD, consistent with NCAM' growth. The contributions to future NCAM' programs which may be anticipated from this action provide an illustrative example of benefits resulting from interactions between the MMRD and NCAM'. Interactions of this type between the two organizations will also increase the contact between NCAM' and the local educational enterprise because of the large fraction of faculty and students associated with the MMRD, a relationship which will surely continue.

The Panel believes that several actions should be taken expeditiously to assure that the materials initiative is pointed in the proper direction from the beginning.

(1) The goals and objectives of the materials initiative should be restated by LBL to clarify its intended technology focus. Included in this statement should be mention of the ALS decoupling and the agreed upon title for the NCAM' initiative.

(2) An NCAM' Director should be appointed as soon as a strong candidate can be identified. The individual chosen for this position must have a thorough understanding of the industrial community and its needs, have experience in managing directed research, and possess requisite scientific credentials. The Director should not be made responsible for ALS planning or operation.

(3) An NCAM' advisory board should be organized, with strong industrial representation, to provide policy guidance.

(4) An acceptable NCAM' program plan should be developed under the NCAM' Director's guidance. This process should begin with a systematic identification of major industrial activities which are seriously constrained by available materials technology.Before any commitments to specific topical areas are made, contributions to the national effort by existing programs at other institutions should also be carefully weighed. To the maximum extent possible NCAM' should strive to develop major roles in a few, carefully chosen, technologically important areas of materials science in which the current national effort is demonstrably inadequate.It is most essential that this planning effort involve strong industry participation.

(5) An organizational structure should be established which fits the NCAM' program objectives. This task should include the definition of an appropriate NCAM'/MMRD interface to assure an effective functional relationship between these organizations. In this connection, careful thought should be given to the possibility of transferring some existing MMRD activities to NCAM' in order to expedite the start-up phase of the new initiative. The Electron Microscopy Center is an example of an MMRD activity which might be examined for possible assignment to NCAM'.

(6) Effective mechanisms for industrial involvement should be implemented. The desired close coupling to the industrial community poses a major challenge and may require organizational concepts and procedures (e.g., funding schemes) not part of LBL's tradition. Existing models which have proven effective elsewhere should be examined for NCAM'

applicability. Among relevant DOE examples, the Sandia Combustion Research Center may be cited; possible university examples include Stanford's Center for Integrated Systems (CIS) and Cornell's National Research and Resource Facility for Submicron Structures (NRRFSS). Careful thought should be given at the outset to matters related to patent rights and proprietary information. Every effort should be made to avoid unnecessary disincentives in this regard for industry involvement in NCAM' research programs. Consideration should also be given to joint DOE/industry funding for appropriate project efforts.

(7) A funding strategy should be developed. Special consideration should be given to integration of ER/BES funding with support from DOE's programmatic organizations (i.e., nuclear, fossil, solar, etc.), as well as industry. Such augmentation of BES resources would strenthen the technology focus and promote more effective program balance between fundamental and applied research. It would also assure that the program objectives remain consistent with DOE's mainline responsibilities, thereby strengthening the NCAM' claim to a DOE mission designation. Nevertheless, a single program office in DOE should be given oversight responsibility for NCAM', together with the requisite authority to prevent destabilizing effects of multiple funding sources and to assure balance and cohesion among various program elements. Since the core effort will be funded by the Materials Sciences Directorate of BES, that office is the appropriate choice for this assignment.

(8) A staffing strategy should be developed. The Panel views staffing to be a critical obstacle to successful implementation of the NCAM' concept. A highly motivated, technically superior professional staff is essential. The excellence of the MMRD is built largely (though not entirely) on UC faculty. Unfortunately, this LBL tradition will not serve the NCAM' needs. In the first place, only a limited number of faculty appointments will be available in the near term to support NCAM' growth. In the second place, it is highly doubtful that a directed, goal-oriented program as described here can be conducted with a staff which is dominated by university faculty, students and postdoctoral fellows. A major challenge will therefore be to attract and retain a sufficient number of senior staff without the inducement of faculty appointments. The Panel hopes that staff additions for NCAM' programs can be satisfied to a large extent by outstanding individuals sufficiently early in their careers that faculty appointments are not likely to be a significant issue. The Berkeley reputation for scientific excellence should be helpful in recruiting such first-rate talent. Nevertheless, the creation of a climate at LBL in which professional status in the materials-sciences field is not equated to faculty appointments must be viewed as a fundamental management problem.

(C) ALS and the SSRL Improvements

The Panel recognizes the important role of synchrotron radiation in a wide variety of scientific investigations. Indeed, it expects that advanced light sources with higher

brightness and different time structures will be required for future research. However, as stated earlier, the ALS is not judged by this Panel to be an appropriate centerpiece for an advanced materials initiative. Rather, it should be considered on its own merits. An evaluation of the ALS based on broader user interests must await a separate review involving the national synchrotron radiation community, especially since the Panel is not in a position to take a definitive stand on three crucial issues affecting the ALS decision:

(1) Urgency of another synchrotron source at this time.
(2) Choice between VUV and hard x-rays for the next light source.
(3) Near-term technical feasibility of a light source capable of attaining the specified ALS operating characteristics in a reliable, reproducible manner.

As concerns the time-urgency question, the Panel believes that the argument revolves less around the need for an increased number of synchrotron-radiation beam lines than around the increased utility of synchrotron radiation with qualitatively different characteristics -- in the present case, significantly shorter pulse durations and/or higher spectral brightness. History suggests that new measurement capabilities usually stimulate unexpected scientific advances. The value judgment should, of course, be left to the user community.

If a decision is made subsequently to proceed with an advanced VUV/soft x-ray facility, its location at LBL would be a sound choice. The following considerations contributed to this view:

(1) LBL's record of accomplishment in the development of insertion-device technology.
(2) LBL's outstanding accelerator science and engineering staff.

40-574 O - 85 - 66

(3) The assured availability of LBL support facilities.

(4) A west coast location of a major VUV/soft x-ray facility would contribute a greater geographic balance to the national synchrotron effort; with the complementary SSRL emphasis on hard x-rays, a balanced west coast synchrotron user complex would be created.

Regardless of when or how a final decision on the ALS is reached, LBL should continue to pursue the following tasks:

(1) Since the ALS represents an advance in electron storage-ring technology and will produce synchrotron radiation with very high spectral brightness and very short pulse lengths, additional facility R&D is desirable to minimize design uncertainties. This includes design studies on insertion devices, optical materials and components, and the proper choice of vacuum-tank material. Short-bunch-length phenomena should be studied. Also, the impact of the proposed superconducting wiggler on the performance of the other insertion devices should be evaluated further.

(2) Develop a broader community of potential users and quantify their needs.

(3) Explore design alternatives aimed at lower cost, and greater responsiveness to user community interests as judged by recent workshops and future interactions.

All of these activities are of considerable general interest, and promise to benefit the future of synchrotron-radiation research independent of the ALS decision. The Panel believes that support should therefore be provided for the above mentioned activities.

Should the ALS or a similar facility be located eventually at LBL it would require a resident, core research program for its effective operation as a user facility. Resources for such an activity should not be drawn from NCAM' funding, except to an extent clearly justified by NCAM' program interests. The Panel recognizes that LBL and SSRL both have strengths in the synchrotron-radiation area. Cooperation between these institutions has contributed significantly to capabilities and accomplishments of the SSRL facility. Both groups would benefit from further strengthening of their collaborative efforts, especially in connection with plans for future facility additions and improvements at the two locations. In the meantime, the proposed upgrade of the SSRL facility is strongly supported by the Panel. This support is based on the following reasons:

(1) Within the constraints imposed by current facility limitations, SSRL has established an extensive user community (with participation from industry, universities, and other laboratories), and can point to significant scientific accomplishments.

(2) The existing support facilities at SSRL are marginal in relation to existing needs and opportunities.

(3) Currently available high-quality beam time at SSRL is inadequate to meet user demands.

(4) The opportunity exists to install a hard x-ray beam line of superior characteristics on PEP at relatively modest cost.

VI) Concluding Remarks and Recommended Funding

Successful realization of NCAM' as viewed by this Panel would result in an activity with the following dominant characteristics:

(1) The organization would seek major contributory roles in selected areas and not simply augment or slightly extend the materials R&D efforts now performed elsewhere.

(2) Programs would be supported based on their direct relevance to either major industrial technologies that are now or will in the future be limited by available materials, or strategic-materials interests of the nation which are not being addressed by the private sector.

(3) The organization would serve as a link between appropriate National Laboratory and industrial communities, on one hand, and between academic and industrial communities, on the other.

(4) Program planning and execution would involve significant direct participation by the industrial community, including the commitment of R&D funds to joint efforts.

Decisions concerning future growth and maximum size of NCAM' should be based on LBL's progress toward establishing programs having the recommended character. Assuming complete success, the Panel envisions an NCAM' enterprise comprising a total technical staff of perhaps a few hundred at steady state, requiring an annual operating budget (derived from several sources) in the range of $30-50M. This estimate was derived from knowledge concerning comparable directed-research activities at other institutions and the expectation that a successful NCAM' would eventually develop 2-4 areas of concentration in addition to the initial catalysis effort.

Because of the subjective nature of these considerations, the size projection is, of course, subject to some uncertainty. An effort of this magnitude would constitute a measurable redirection of LBL and would also be of sufficient magnitude to qualify the activity as a serious attempt to pioneer a new mode of materials research in a DOE National Laboratory. How useful the experience gained in establishing NCAM' will be to other laboratories, however, remains to be determined. The close association of LBL with UC/Berkeley creates opportunities, as well as problems, which are not in most instances encountered by other federal laboratories. For example, the major-university setting of LBL offers outstanding opportunities for technical interactions with world-class scientific talent. On the other hand, successful implementation of NCAM' at LBL is likely to encounter staffing and management problems peculiar to that institution. These would be much less serious at Laboratories where traditions are more closely related to industrial models.

The FY-84 funding to support the Panel's recommendations totals $22.5M ($13.4M for construction and $9.1M for operating and equipment). Details are shown in Appendix VI. The construction funds would provide $9.3M for LBL's Surface Science and Catalysis Laboratory and $4.1M for the SSRL upgrade. The recommended SSRL construction funds include $0.3M for the 18° beam-line project which the original NCAM proposal had included in the ALS line item, as indicated in Appendix III. The operating/equipment funds would support continued development of synchrotron-radiation technology, provide modest initial growth for the surface-science/catalysis program, and provide a total of $2.0M for NCAM' program planning and 'seed money' to initiate necessary staff hiring program in support of future NCAM' activities. <u>While the Panel favors continued support for R&D on advanced light sources at LBL, the decision</u>

whether or not to proceed with actual construction of an ALS should await completion of a synchrotron-radiation community review, as discussed previously in this report.

The FY-85 funding requirements include construction funds to assure rapid completion of the SSCL and SSRL/SEPFF projects. The Panel also supports the $12.7M request for operating and equipment as detailed in Appendix III. However, whether commitment of design funds for the AMSL/ADCL facility will be justified in FY-85 cannot be determined by the Panel at this time. A final decision should be contingent on progress by the NCAM' team during coming months, especially in regard to program planning. The above-stated requirement for an independent ALS review applies to FY-85 construction-funding considerations, as well.

As the Panel was finishing its deliberations, it learned that the FY-84 Energy and Water Development appropriation bill, while including the requested operating and equipment funds for NCAM, contained only $3.0M for NCAM construction. The Panel believes that this action may force undesirable delays during the crucial formative stages of the NCAM' initiate, thereby reducing the probability of it ever being implemented successfully. For this reason the Panel hopes that it will be possible to increase the FY-84 construction funding to permit, at a minimum, start of construction of the SSCL and support of the 18° beam line project at SSRL.

APPENDIX I

Department of Energy
Washington, D.C. 20585

MAR 31 1983

Dr. Albert Narath
Executive Vice President
Sandia National Laboratory
P. O. Box 5800
Albuquerque, New Mexico 87185

Dear Al:

I appreciate your willingness to undertake the task of serving as Chairman of an ad hoc panel to review the technical and programmatic aspects of the National Center for Advanced Materials (NCAM) at the Lawrence Berkeley Laboratory. Prior to outlining the elements that I expect to be included in your review, it might be helpful to mention some of the events that motivated the establishment of this Center.

The decision to establish the Center was based on many considerations. Some of these came from the recommendations made by the Energy Research Advisory Board's Multipurpose Laboratory Review Panel: That the Department should seek to redirect its laboratories into new and scientifically more productive activities, that it use its laboratories in ways that support the Nation's higher education enterprise, that it seek to get them more involved with industry in ways that help improve the U.S. industrial science and technology base, and finally, that it not regard its laboratories simply as sites at which various unrelated technical projects are performed for the different departmental elements, but rather regard the laboratories, to the extent possible, as institutions and treat them accordingly.

Each major multiprogram laboratory annually submits an institutional plan to the Department. In this plan, the laboratory identifies its long range plans with respect to ongoing activities as well as any new activities that it believes might make better use of existing facilities and skills to work on problems associated with the Department's missions. In its 1983 plan, the Lawrence Berkeley Laboratory proposed to establish a National Center for Advanced Materials.

The Center would feature several state-of-the-art instruments and facilities related to the study of materials; some of this capability currently exists. A new synchrotron light source with very high brightness and making extensive use of insertion devices would comprise the core facility. The Center and its associated program would focus some of the activities at Berkeley on materials science in a way that would enhance the research competence of the staff, train students in this important area, and involve industrial and university users in scientific projects in novel modes that should promote more rapid effective technology transfer from basic materials research to industrial applications.

With respect to the specific tasks for the Panel, your review should include a thorough examination of all the elements and activities proposed for the Center. This should involve a technical review of the various proposed facilities, their cost, and their appropriateness to their proposed purposes. Also, it should include a programmatic review of the proposed organizational arrangements, the establishment and charters for standing advisory mechanisms, and the plans for the involvement of and interaction with U.S. industry. The plans for interaction with other national laboratories and universities should also be examined with respect to their completeness and expected effectiveness. The Panel may well have other issues that it wishes to explore in connection with the proposed activities.

I wish to make clear at the outset that a revisitation of the Department's basic decision to establish this Center, with its associated facilities, is not being requested. That decision was made on the basis of broad institutional concerns in the context of a widely accepted need for enhanced national effort in this area of science. Instead, the Panel's purpose is to critique and improve the initial LBL planning so that the best possible features and activities for this facility are incorporated during this early phase while it is still possible to make changes and improvements without incurring additional costs.

As I indicated in my testimony to several congressional committees this year, I am aware that concerns and constructive suggestions have been expressed by members of the U.S. science and education communities regarding the establishment of this Center. I expect the Panel to hear the views of as many of those who are concerned as is appropriate. The number of individuals to involve is obviously a matter of judgement for you and the Panel, but in any case, I hope that potential users of these facilities in the various fields of science all have a fair hearing.

I have asked Dr. Donald Stevens, Deputy Associate Director of the Office of Basic Energy Sciences, to serve as Executive Secretary for the Panel and to arrange any backup assistance you may require from the Department.

I plan to attend the Panel's first meeting at Berkeley and would be pleased to discuss any matters pertaining to the Department's position on the Center.

This is an important task and involves more than a simple technical review. This proposed Center should serve as a model for activities at other national laboratories that would improve their effectiveness in helping the United States maintain its scientific and technological leadership. This is why the Panel members have been chosen from industry, university and laboratories, not only for their technical expertise, but also for their ability to have a long range view of this proposed activity and its importance to our nation.

Although I don't wish to hurry you in any way that might cause the Panel to leave any loose ends, I would hope that you could arrange the necessary meetings and deliver your report to me by the end of August 1983.

Sincerely,

Alvin W. Trivelpiece
Director, Office of
Energy Research

APPENDIX II

A. Narath
Executive Vice President

Sandia National Laboratories
Albuquerque, New Mexico 87185

June 10, 1983

Dr. Alvin W. Trivelpiece
Director
Office of Energy Research
U. S. Department of Energy
Washington, D.C. 20585

Dear Al:

You asked that I document the principal findings which are emerging from the review being conducted by the ad hoc NCAM Panel. You expressed particular interest in the Panel's views regarding FY-84 funding requirements.

To date the NCAM Panel has held two meetings, one in Berkeley for an extensive briefing by LBL management and staff and a second one in Washington for interviews with senior members of the materials-science community representing a broad spectrum of interests. Furthermore, individual Panel members have discussed the NCAM proposal with additional prominent materials scientists, reviewed other relevant information, and attended the LBL synchrotron radiation workshop. These activities have led to the following assessment:

(1) The establishment of a new materials initiative at LBL characterized by a strong technology focus offers exciting opportunities for significant advances in this important field. A structured, "technology-pull" effort would build on and complement existing strengths in LBL's MMRD (Materials and Molecular Research Division) with its more traditional unstructured, "basic-research push" orientation.

(2) It is possible that the ALS (Advanced Light Source) may be justified as a "next generation" VUV/soft x-ray user facility to complement the Stanford SSRL x-ray source capabilities. Assuming continued user pressure for increased numbers of beam lines, this combination of facilities could evolve into a major regional (western) user-oriented research center for spectroscopic research. We acknowledge the fact that synchrotron radiation has become one of several important tools in materials science research. Nevertheless, the ALS cannot in our view be justified

solely as an essential element in a technology-oriented materials initiative. It should, therefore, be decoupled from the proposed materials program and considered on its own merits.

Two steps should be taken as expeditiously as possible in support of the materials initiative. (1) Appointment of a Director to organize the initial effort around existing capabilities and to develop a program plan to justify and guide future growth. The individual chosen for this position should understand the industrial community and their needs, know how to manage research, and meet required scientific standards. (2) Funding ($9.3M) for construction of the SSCL (Surface Science and Catalysis Laboratory) beginning early in FY 84. LBL has unique strengths in these fields and an immediate expansion of the program to address technologically significant objectives is fully justified. Such a step would also signal a crucial commitment to the initiative without which it would be very difficult to launch this enterprise.

In regard to the ALS, several tasks must be pursued before a firm commitment to this facility should be contemplated. (1) Establishment of a user community more broadly-based than was encouraged by the previous tight coupling to the materials initiative. The recent workshop was only the first step toward collecting appropriate user input. The biological community participation is still disappointingly small. (2) Consideration of ALS design alternatives with the objective of satisfying ultimate user needs, while minimizing cost. (3) Continued R&D on specific technical issues relevant to the design of a "next-generation" synchrotron light source.

In the meantime there is considerable urgency to provide the requested funding ($4.1M) to permit initiation of the Stanford SSRL improvements. User demands for this x-ray facility greatly exceed current capabilities. This situation would be relieved considerably by the proposed upgrade of SPEAR and associated support facilities. The cost is modest in relation to the benefit.

In summary, we strongly urge that construction funding of $13.4M (compared to the original request of $25.9M) be supported in FY 84.

Best regards,

A. Narath
Chairman, Ad hoc NCAM Panel

APPENDIX III

National Center for Advanced Materials Funding Profile

(Obligations, Actual Year $M)[a]

	FY83	FY84	FY85	FY86	FY87	FY88	FY89	Total FY84-89	
OPERATING R&D									
1. ALS R&D	0.95	1.3	1.9	0.6	0.3	--	--	4.1	
2. Source & Optical R&D	0.40	2.1	2.5	1.2	1.0	--	--	6.8	
3. Capital Equipment	0.30	0.5	0.4	0.4	0.7	--	--	2.0	
4. ALS Pre-Operation/Operations	---	---	--	--	2.5	7.0	13.5	23.0	
5. SSRL	--	0.7	0.7	--	--	--	--	1.4	
Subtotal, Operations/R&D	1.65	4.6	5.5	2.2	4.5	7.0	13.5	37.3	
PROGRAMMATIC RESEARCH[b]									
6. Surface Science & Catalysis									
Operating	--	1.1	2.0	4.4	6.0	7.4	8.8	29.7	
Capital Equipment	--	0.4	0.6	0.9	1.2	1.5	2.2	6.8	
7. Advanced Materials Synthesis									
Operating	--	1.4	1.8	3.3	4.8	6.9	8.8	27.0	
Capital Equipment	--	0.7	0.8	0.6	1.0	1.2	2.2	6.5	
8. Advanced Device Concepts									
Operating	--	0.6	1.1	2.1	2.5	3.8	5.3	15.4	
Capital Equipment	--	0.3	0.9	0.4	0.5	1.0	1.2	4.3	
Subtotal, Programmatic Research	--	4.5	7.2	11.7	16.0	21.8	28.5	89.7	
CONSTRUCTION									
9. Advanced Light Source	--	11.6[d]	18.8	19.9	15.0	13.5	5.3	84.1	
10. Surface Science & Catalysis Lab	--	9.3	0.9	0.7	--	--		10.9	
11. Advanced Materials Synthesis/ Advanced Device Concepts Lab	--	1.2	1.3	2.8	14.4	9.8	1.7	31.2	
12. SEPFF[c]	--	3.8	5.6	3.3	--	--		12.7	
Subtotal, Construction	--	25.9	26.6	26.7	29.4	23.3	7.0	138.9	(TEC)
TOTAL	1.65	35.0	39.3	40.6	49.9	52.1	49.0		

a 10% Annual inflation included.
b Increment above present programs.
c SSRL Extended Photon Flux Facility
d Includes $0.3M for 18° beam line at SSRL

APPENDIX IV

The Inorganic Materials Research Division (IMRD, predecessor to MMRD) was organized at LBL in 1961 by the Atomic Energy Commission (AEC) as part of a federal program to establish interdisciplinary materials research laboratories (IDL's) at universities. The AEC also established a major IDL at the University of Illinois. The Department of Defense, through its Advanced Reseach Projects Agency (ARPA) established twelve IDL's (including one at Illinois also) of varying size and the National Aeronautics and Space Administration NASA) established two. The National Science Foundation (NSF) chose not to participate in the program; but in 1972 ARPA transferred its 12 projects to NSF which then established 4 additional IDL's. The goals of the program were to (1) increase the rate of manpower training in the materials sciences, (2) promote interdisciplinary interactions in this field in hopes of upgrading certain topics (such as ceramics) and encouraging new materials concepts, and (3) expand the national basic research effort in the materials sciences.

The AEC chose U.C. Berkeley and the University of Illinois because of the large number of research projects in the fields of metallurgy, ceramics, and solid-state physics that it supported on these campuses. At Berkeley, the AEC bought up other agency contracts and grants supporting faculty conducting metallurgical and ceramic research, and merged this group administratively with professors, mainly chemists, who were receiving their research support through LBL. The metallurgists and ceramists were conducting basic research in ferrous metallurgy, dislocation theory and the influence of dislocations on mechanical properties, sintering, metal-ceramic interfaces, theory of creep and deformation, and high-temperature compounds (silicides and germanides), as examples.

The chemists were conducting research in fields such as chemical thermodynamics, phase diagrams, high temperature chemistry, high pressure phenomena, electrochemistry and surface reactions. When the merger was completed and other agency contracts and grants were phased out in 1963, the newly formed Inorganic Materials Research Division was equally supported by AEC materials and chemistry program offices at a total annual level of approximately $2.2M. Most of the research was conducted on the Berkeley campus and remained integrated into the graduate programs of the University. The first Head of the IMRD was Dr. L. Brewer.

In 1965 the LBL Laboratory Building 62 was completed. It provided new research laboratory space for about half of the Division's staff. In 1974 an unsuccessful proposal was made for an addition to the laboratory building and for funds to establish a center for engineering materials research. It was during this period (1965-1975) that research on surfaces gained substantial momentum. Also, transformation induced plasticity in steels (TRIP steel) was invented and patented. The latter work involved substantial interaction with the steel industry.

In 1975 the name of the Division was changed to the Materials and Molecular Research Division, Dr. D. A. Shirley was named Head and a number of additional LBL chemists were transferred into the organization. Emphasis on ferrous metallurgy and metal phase diagrams diminished due to retirements and loss of senior staff while emphasis on electron microscopy, ceramics, surface phenomena (corrosion, erosion, and surface structure), catalysis, and research using synchrotron radiation and molecular beams increased. At the same time, solid-state and theoretical physicists in the U.C. Berkeley Physics Department were attracted into the program. In the later 1970's funds

were provided for the purchase of a 1.5 MeV electron microscope to replace the aging 650 keV machine that had been acquired in 1969. In 1980 and 1981 the Department of Energy included requests for funds to acquire an atomic-resolution electron-microscopy facility, and to build a surface-science laboratory addition to the MMRD building. The Congress only provided sufficient funds for the microscopy facility, and design funds for the surface science laboratory. Finally, to complete this historical sketch, in 1980 Dr. Shirley was named Director of LBL and Dr. A. W. Searcy succeeded him as Head of the MMRD.

While the activities of the MMRD have diversified substantially since its formation in the early 1960's, heavy emphasis continues on basic materials and materials-related research. The FY-83 operating budget for the MMRD is as follows:

		K$
Energy Research:	Materials Sciences	$ 7,270
	Chemical Sciences	4,432
	Nuclear Sciences	1,172
	Magnetic Fusion Energy	150
Fossil Energy		600
Energy Storage		1,220
Work for Others*		605
	TOTAL	$15,449

*ORNL, Battelle Northwest, LANL, LLNL, Detroit Diesel, ONR, NASA, etc.

In 1982, 29 M.S. degrees and 55 Ph.D. degrees were awarded to graduate students whose thesis research studies were supported by the MMRD.

Many major awards in materials sciences, chemistry, solid-state physics and related engineering fields have been won by current

MMRD investigators; for example, the Baekeland Award, Award in Industrial and Engineering Chemistry, Pollution Control Award, Award in Inorganic Chemistry, the Priestly, Lewis, Gibbs Awards, Award in Pure Chemistry, Award in Colloid and Surface Chemistry, and the Award in Petroleum Chemistry, all of the American Chemical Society; the Matthey, Purdy, Sosman, Fulrath, and Jeppson Awards of the American Ceramics Society; the Hardy, Extractive Metallurgy-Science, Hume-Rothery, Stoughton, and Mathewson Awards of AIME; the Colburn, Walker, and Professional Progress Awards of the American Society of Chemical Engineers; the Acheson Award and Palladium Medal of the Electrochemical Society, the Buckley Prize in Solid-State Physics. Glenn Seaborg is the recipient of the Nobel Prize in Chemistry, the Fermi Award and numerous other awards and honorary degrees. The current staff of MMRD includes 13 members of the National Academy of Science, 7 members of the National Academy of Engineering, and one member of the Royal Society of London. Four Lawrence Awards and 26 Guggenheim Fellowships have been given to current staff.

APPENDIX V

TABLE OF CONTENTS

of the

MATERIALS AND MOLECULAR RESEARCH DIVISION

ANNUAL REPORT 1982

40-574 O - 85 - 67

Contents

GENERAL INTRODUCTION xxiii

I. MATERIALS SCIENCES
A. Metallurgy and Ceramics
1. Structure of Materials

a. Structure and Properties of Transformation Interfaces
Ronald Gronsky, Investigator

1. Grain Boundaries in Body-Centered Cubic Metals 1
2. Grain Boundaries and Interfaces in Semiconductors 2
3. Transformation Interfaces in Aluminum Alloys 2

1982 Publications and Reports 3

b. Microstructure, Properties, Alloy Design: Inorganic Materials
Gareth Thomas, Investigator

A. Alloy Design: Medium Carbon Steels

1. Characterization of the Effects of Laser Heat-Treatment Upon the Microstructure and Mechanical Properties of Fe/3Cr/2Mn/0.5Mo/0.3C 4
2. Mechanical Properties and Microstructure of Lower Bainite in a 0.3%C-3%Cr-2%Mn Steel 5
3. The Nature and Origin of Sliding Wear Debris from Steels 5
4. Fundamentals of Abrasive Wear 6

B. Alloy Design: Low-Carbon Dual Phase Steels

1. Design of High Strength Dual-Phase Steel Wire 6

C. Magnetic Materials

1. EM Study of CaO Segregation at the Grain Boundaries in $(Mn,Zn)Fe_2O_4$ 7
2. Development of the Cellular Microstructure in the $SmCo_{7.4}$-Type Magnets 8
3. Electron Microscopy of Mn-Al Magnets 8
4. Annealing of High Permeability $(Mn,Zn)Fe_2O_4$ 9

1982 Publications and Reports 9

c. Solid State Phase Transformation Mechanisms
Kenneth H. Westmacott, Investigator

1. Precipitation in the Pt-C System 11
2. Ledge Structure and Precipitate Growth in Al-Cu 11
3. The Relationship Between Invariant Line Strain and Precipitate Needle Growth 11
4. Mo_2C Precipitate Structure and Morphology in Molybdenum 12
5. Work in Progress 13

1982 Publications and Reports 13

d. National Center for Electron Microscopy
Gareth Thomas, Ronald Gronsky, and
Kenneth H. Westmacott, Investigators

1. 1.5 MeV High Voltage Electron Microscope 14
2. Atomic Resolution Microscope 19
3. Periodic Extension in Optical Diffraction Analysis 20
4. Real Space Image Simulation in High Resolution Microscopy 20
5. Characterization of AlN Ceramics Containing Long Period Polytypoids 21

1982 Publications and Reports 21

e. In-Situ Investigations of Gas-Solid Reactions by Electron Microscopy
James W. Evans and Kenneth H. Westmacott, Investigators

1. The Microstructure and Reactivity of Metal Oxides 22

1982 Publications and Reports 24

f. Local Atomic Configurations in Solid Solutions
Didier de Fontaine, Investigator

1. Long-Period Superstructures 25
2. TTT Diagrams 25

1982 Publications and Reports 26

2. Mechanical Properties

a. Theoretical Problems in Alloy Design
John W. Morris, Jr., Investigator

1. The Linear Elastic Theory of Phase Transformations in Solids 27
2. Dislocation Motion at Low Temperature 27
3. Microstructural Sources of the Ductile-To-Brittle Transition in Steel 28
4. The Coupling Between Magnetic- and Deformation-Induced Martensite in Metastable Austenitic Steels 29
5. Mössbauer Spectrometry 29
6. The Metallurgy of Fe-Mn Steels 29
7. High Temperature Embrittlement of an Iron-Based Superalloy 30
8. Microstructure Control During Welding of Ferritic Steels 30
9. Superalloy Welding 30
10. The Use of Heat Treatment to Improve the Critical Current of Bronze-Process Multifilamentary Superconducting Wire 31
11. The Influence of Magnesium Additions on the Properties of Multifilamentary Nb_3Sn Superconducting Wire 31

1982 Publications and Reports 32

b. Mechanical Properties of Ceramics
Anthony G. Evans, Investigator

High Temperature Failure

1. High Temperature Failure Initiation in Liquid Phase Sintered Materials 34
2. A Damage Model of Creep Crack Growth in Polycrystals 34
3. High Crack Growth in Polycrystalline Alumina 35
4. The Influence of Inhomogeneities on High Temperature Failure in Ceramics 35

Sintering

1. Microstructure Evolution During Sintering: The Role of Evaporation/Condensation 36

2. An Experimental Assessment of Pore Breakaway During Sintering 36
3. Initial Stage Sintering with Coupled Grain Boundary and Surface Diffusion 37

1982 Publications and Reports 37

c. Environmentally Affected Crack Growth in Engineering Materials
Robert O. Ritchie, Investigator

1. On the Load Ratio Dependence of Fatigue Thresholds 39
2. Influence of Viscous Environments on Fatigue Crack Growth 40
3. Fatigue Resistant Microstructures in Dual-Phase Steels 40
4. Mechanisms of Fatigue Crack Growth Under Variable Amplitude Loading 40

1982 Publications and Reports 40

3. Physical Properties

a. Interfaces and Ceramic Microstructures
Joseph A. Pask, Investigator

1. Wetting and Reactions in the Lead Borosilicate Glass-Precious Metal Systems 43
2. The Silica-Alumina System 43

1982 Publications and Reports 44

b. High Temperature Reactions
Alan W. Searcy, Investigator

1. The Equilibrium Shapes of Crystals and of Cavities in Crystals 45
2. Effects of Particle Size and Powder Bed Size on Calcite Decomposition Rates 45
3. Possible Metastability of MgO Resulting From the Decomposition of $Mg(OH)_2$ 46
4. Confirmation of Bimodal Pore Size Distribution in CaO from Calcite Decomposition 47
5. Gas Flow Through Porous Barriers: The O_2-Pt, CO-Pt Systems 47

1982 Publications and Reports 48

c. Structure-Property Relationships in Semiconductor Materials
Jack Washburn, Investigator

1. The Mechanism of Degradation of Cu_2S-CdS Solar Cells as Revealed by High Resolution Electron Microscopy 49
2. An Application of High Resolution Lattice Imaging Electron Microscopy to a Study of the Mechanism of the Crystalline to Amorphous Transformation 49
3. Effect of Recoil Implanted Oxygen on the Development of Secondary Defects in MOS Test Wafers 50
4. In-Situ Observations of MeV Electron Beam Induced Crystal Growth into an Amorphous Layer in Silicon 50
5. Effect of Temperature and Displacement Damage on the Growth of Amorphous Layers in Silicon 50
6. A Model for Redistribution of Phosphorus During Annealing of High Dose Ion Implanted Silicon 51
7. Diffraction Extinction Conditions for Silicon and Other Materials with Diamond Glide Planes 51

1982 Publications and Reports 52

d. Chemical Properties and Processing of Refractory Ceramics
Lutgard C. De Jonghe, Investigator

1. Processing of Ceramics 53
2. Structure and Nonstoichiometry of Calcium Aluminates 53
3. Work in Progress 55

1982 Publications and Reports 55

e. Structure and Electrical Properties of Composite Materials
Robert H. Bragg, Investigator

1. Density of Heat-Treated GC 56
2. Pore Growth in Glassy Carbon 57
3. Work in Progress 57

1982 Publications and Reports 57

f. High Temperature Oxidation and Corrosion of Materials
David P. Whittle, Investigator

1. Mechanism of Peg Growth and Influence on Scale Adhesion 58
2. Microstructure and Growth of Protective Cr_2O_3 and Al_2O_3 Scales at High Temperature 59
3. The Influence of Alloy Microstructure on Al_2O_3 Peg Morphologies in CoCrAl Alloys and Coatings 60
4. Sulfur Diffusion in Oxide Grain Boundaries 60
5. The Effects of SO_2 and SO_3 on the Na_2SO_4 Induced Corrosion of Nickel 61
6. Effects of Chlorides on Na_2SO_4-Induced Hot Corrosion of MCrAl 61
7. Multiphase Diffusional Growth During Aluminizing 62
8. High Temperature Oxidation of Ni-Co Alloy 62

1982 Publications and Reports 63

g. Ceramic Interfaces
Andreas M. Glaeser, Investigator

1. Grain Boundary Mobility Measurements in MgO-Doped Al_2O_3 64

1982 Publications and Reports 65

4. Engineering Materials

a. Abrasive, Erosive, and Sliding Wear of Materials
Iain Finnie, Investigator

1. Sliding Wear of Dissimilar Metals 66
2. Abrasive Wear 66
3. An Overview of Wear 66

1982 Publications and Reports 67

b. Erosion-Corrosion Wear Program
Alan V. Levy, Investigator

1. Measurement and Numerical Modeling of Two Phase Flow 68
2. Measurements of Air Flow in a Curved Pipe Using Laser-Doppler Velocimetry 68
3. Particle Flow Characteristics Determination in Gas and Liquid-Solid Particle Streams 68

1982 Publications and Reports 69

c. Erosion of Brittle Solids
Anthony G. Evans, Investigator

1. The Mechanical Behavior of Brittle Coatings and Layers 70
2. Measurements of Dynamic Hardness by a Controlled Impact Technique 71

1982 Publications and Reports 71

d. Chemical Degradation of Refractories
David P. Whittle, Investigator

1. High Temperature Degradation of Refractories in Mixed Gas Environments 72

5. Experimental Research

a. Far Infrared Spectroscopy
Paul L. Richards, Investigator

1. Infrared Emission Spectroscopy of CO on Ni 73
2. Low Temperature Infrared Absorption Spectroscopy of CO on Ni 74
3. Far Infrared Optical Properties of an Organic Superconductor 74
4. Work in Progress 74

1982 Publications and Reports 75

b. Experimental Solid State Physics and Quantum Electronics
Yuen-Ron Shen, Investigator

1. Spectroscopy of Molecular Monolayers by Resonant Second-Harmonic Generation 77
2. Transient Four-Wave Mixing and Coherent Transient Optical Phenomena 78
3. Nonlinear Wave Interaction Involving Surface Polaritons 79
4. Surface-Enhanced Second-Harmonic Generation and Raman Scattering 79

1982 Publications and Reports 79

c. Excitations in Solids
Carson D. Jeffries, Investigator

1. Period Doubling and Universal Chaotic Behavior in P-N Junctions in Silicon 82
2. Intermittency Route to Chaos 83
3. Period Doubling and Chaos in Spin Wave Instabilities in Yttrium Iron Garnet 83

1982 Publications and Reports 84

d. Time-Resolved Spectroscopies in Solids
Peter Y. Yu, Investigator

1. Nonequilibrium Phonon Spectroscopy in GaAs 85
2. Lifetime of Ortho-Exciton and Ortho- to Para-Exciton Conversion in Cu_2O 85

1982 Publications and Reports 85

e. Superconductivity, Superconducting Devices, and 1/f Noise
John Clarke, Investigator

1. Chaos in Josephson Junctions 87
2. Measurements of Current Noise in DC SQUIDs 88

3. Correlation Lengths in Magnetotellurics 88

1982 Publications and Reports 89

6. Theoretical Research

a. Theoretical Studies of the Electronic Properties of Solid Surfaces
Leo M. Falicov, Investigator

1. Magnetic and Electronic Properties of Ni Films, Surfaces, and Interfaces 91
2. Thermodynamic Properties of Li Intercalated and Disordered Layer Compounds 92

1982 Publications and Reports 92

b. Theoretical Solid State Physics
Marvin L. Cohen, Investigator

1. Solid Surfaces 94
2. Crystal Structure 94
3. Lattice Dynamics 94
4. Electronic Structure 95
5. Work in Progress 95

1982 Publications and Reports 95

7. Chemical Structure

a. Low Temperature Properties of Materials
Norman E. Phillips, Investigator

1. Absolute Temperature Determinations in the mK Region 97
2. The Specific Heat of ^{3}He in the Fermi Liquid Region 97
3. Low-Temperature Specific Heat of Potassium 98
4. Observation of the Spin Glass-Paramagnet Phase Boundary 98

1982 Publications and Reports 98

b. Electrochemical Processes
Charles W. Tobias, Investigator

1. Anodic Processes in Propylene Carbonate 100
2. Work in Progress 101

1982 Publications and Reports 101

8. High Temperature and Surface Chemistry

a. High Temperature Thermodynamics
Leo Brewer, Investigator

1. Use of Gaseous-Condensed Phase Equilibration to Determine Thermodynamic Quantities for Very Stable Transition Metal Alloys 103
2. High Temperature EMF Measurements 104

1982 Publications and Reports 104

b. Chemistry and Materials Problems in Energy Production Technologies
D. R. Olander, Investigator

1. The UO_2 - Zircaloy Chemical Interaction 106
2. Investigation of Iron-Chlorine Reaction by Modulated Molecular Beam Mass Spectrometry 107

3. A Thermodynamic Assessment of In-Reactor Iodine SCC of Zircaloy 107
4. Multiphoton Laser Ionization Mass Spectrometry of CsI and I 107
5. The Kinetics of Gas/Solid/Liquid Reactions by Modulated Molecular Beam Mass Spectrometry 108

1982 Publications and Reports 108

c. Plasma Enhanced Deposition of Thin Films
Dennis W. Hess, Investigator

1. Plasma-Deposited Titanium Oxide Photoanodes 110
2. Structure and Photoelectrochemical Properties of Plasma-Deposited Iron Oxide Films 110

1982 Publications and Reports 110

d. Electrochemical Phase Boundaries
Rolf H. Muller, Investigator

1. Nucleation of Pb Electrodeposits on Ag and Cu 112
2. Effect of Rhodamine-B on Pb Electrodeposition on Ag and Cu 112
3. Self-Compensating Spectroscopic Ellipsometer 113
4. Work in Progress . . . . . .

1982 Publications and Reports 113

e. Solid State and Surface Reactions
Gabor A. Somorjai, Investigator

Surface Structure and Chemisorption by Low Energy Electron Diffraction and Electron Spectroscopy

1. A LEED Crystallography Study of the (2x2)-C_2H_3 Structure Obtained After Ethylene Adsorption on Rh(111) 115
2. Evidence for the Formation of Stable Alkylidyne Structures From C_3 and C_4 Unsaturated Hydrocarbons Adsorbed on the Pt(111) Single Crystal Surface 115
3. Force-Field Calculations of the Packing Energy of Monolayers of C_3 and C_4 Hydrocarbon Molecules Adsorbed on Single Crystal Metal Surfaces 115
4. Vibrational Studies of Alkene Decomposition on the Rh(111) Surface 116
5. A Covalent Model for the Bonding of Adsorbed Hydrocarbon Fragments on the (111) Face of Platinum 116
6. The Adsorption of Benzene and Naphthalene on the Rh(111) Surface: A LEED, AES, and TDS Study 116
7. Vibrational Spectroscopy Using HREELS of Benzene Adsorbed on the Rh(111) Crystal Surface 116
8. The Structure of Graphitic Carbon on Pt(111) 117
9. The Coadsorption of Potassium and CO on the Pt(111) Crystal Surface: A TDS, HREELS, and UPS Study 117
10. The Interaction of Potassium with π-Electron Orbital Containing Molecules on Pt(111) 117
11. The Characterization of Pt/Cu Alloy and Epitaxial Surfaces 117
12. A New Model for CO Ordering at High Coverages on Low Index Metal Surfaces: A Correlation Between LEED, HREELS, and IRS. CO Adsorbed on fcc (100) Surfaces 118
13. LEED Intensity Analysis of the (1 x 5) Reconstruction of Ir(100) 118
14. The Adsorption and Binding of Thiophene, Butene, and H_2S on the Basal Plane of MoS_2 Single Crystals 118
15. LEED and AES Study of Zirconium Overlayers on the Pt(100) Crystal Face 118

Studies of Catalyzed Surface Reactions

1. Ammonia Synthesis Catalyzed by Rhenium 119

2. Interaction of CO, CO_2, and D_2 with Rhodium Oxide: Its Reduction and Catalytic Stability 119
3. Deuterium Isotope Effects for Hydrocarbon Reactions Catalyzed Over Platinum Single Crystal Surfaces 119
4. Studies of Sulfur Monolayers on Mo(100) and Its Effects on Adsorbate Binding 119
5. The Effect of Potassium on the Catalyzed Reactions of n-Hexane Over Pt(111) and Pt-[6(111)x(111)] Single Crystal Surfaces 119
6. Dehydrogenation of Cyclohexane Catalyzed by Bimetallic Au-Pt Single Crystal Surfaces 120
7. Energy Redistribution Among Internal States of Nitric Oxide Molecules Upon Scattering From Pt(111) Crystal Surface 120

1982 Publications and Reports 120

f. Nuclear Magnetic Resonance
Alexander Pines, Investigator

1. Broadband Population Inversion 124
2. Time-Resolved Optical Nuclear Polarization 124
3. Zero Field NMR 124
4. Anisotropic Diffusion in Oriented Systems 125
5. High Resolution NMR of Feldspars and Zeolites 125
6. Theory of Spin Diffusion in Solids 125
7. Time-Resolved CIDNP and Magnetic Isotope Effect 125
8. Molecular Conformation in Liquid Crystals 125
9. Excitation of High N-Quantum Transitions 126

1982 Publications and Reports 126

II. CHEMICAL SCIENCES
A. Fundamental Interactions
1. Photochemical and Radiation Sciences

a. Photon-Assisted Surface Reactions, Materials, and Mechanisms
Gabor A. Somorjai, Investigator

1. Photocatalytic Production of Hydrogen from Water by a p- and n-Type Polycrystalline Iron Oxide Assembly 129
2. The Preparation and Selected Properties of Mg-Doped p-Type Iron Oxide as a Photocathode for the Photoelectrolysis of Water Using Visible Light 129
3. Work in Progress 129

1982 Publications and Reports 130

b. Photochemistry of Materials in the Stratosphere
Harold S. Johnston, Investigator

1. The Reaction of Chlorine Atoms with Nitric Acid Vapor 131
2. Temperature-Dependent Ultraviolet Absorption Spectrum of Di-Nitrogen Pentoxide 131
3. Work in Progress 132

1982 Publications and Reports 132

2. Chemical Physics

a. Energy Transfer and Structural Studies of Molecules on Surfaces
Charles B. Harris, Investigator

1. Enhanced Photochemistry on Metal Surfaces 133
2. Electronic Energy Transfer to Semiconductor Surfaces 133
3. Vibrational Coherence and Picosecond Studies in Liquids 134

1982 Publications and Reports 134

b. Molecular Beam Spectroscopy
John S. Winn, Investigator

1. Dissociation Mechanisms of Metal Carbonyls 136
2. Supersonic Molecular Beam Relaxation Mechanisms 136

1982 Publications and Reports 137

c. Selective Photochemistry
C. Bradley Moore, Investigator

1. Absolute Rate Constants for the Removal of CH_2 ($^1A_1$). 138
2. High Vibrational Overtone Photochemistry 139

1982 Publications and Reports 140

d. Physical Chemistry with Emphasis on Thermodynamic Properties
Kenneth S. Pitzer, Investigator

1. Relativistic Ab Initio Molecular Structure Calculations Including Configuration Interaction with Application to Six States of TlH 141
2. Electron Structure Calculations Including CI for Ten Low Lying States of Pb_2 and Sn_2. Partition Function and Dissociation Energy of Sn_2 141
3. Nuclear Spin Statistics of Cubane and Icosahedral Borohydride Ions 142

1982 Publications and Reports 142

e. Molecular Interactions
William A. Lester, Jr., Investigator

1. Theoretical Study of Elementary Reactions in Combustion Processes 144
2. Theory of Polyatomic Photodissociation 145
3. Fixed-Node Quantum Monte Carlo for Molecules 146
4. Work in Progress 146

1982 Publications and Reports 146

f. Theory of Atomic and Molecular Collision Processes
William H. Miller, Investigator

1. Dynamical Models for Polyatomic Reaction Dynamics 148
2. Dynamical Effects of Reaction Path Symmetry; Mode-Specificity in the Unimolecular Dissociation of Formaldehyde 148

1982 Publications and Reports 149

g. Photoelectron Spectroscopy
David A. Shirley, Investigator

1. Direct Surface Structure Determination with Photoelectron Diffraction 151
2. High Resolution Fourier Analysis with Auto-Regressive Linear Prediction 151
3. Normal Photoelectron Diffraction of O/Cu(001): A Surface Structural Determination 152
4. The Two-Dimensional Valence Electronic Structure of a Monolayer of Ag on Cu(001) 152
5. The Evolution to Three-Dimensional Valence Band Structure in Ag Overlayers on Cu(001) 153
6. High Resolution Angle-Resolved Photoemission Study of the Valence Band Structure of Ag(111) 154

7. Construction of a High Resolution Electron Energy Loss Spectrometer 154
8. Threshold Measurements of the K-Shell Photoelectron Satellites in Ne and Ar 155
9. Photoelectron Measurements of the Mercury 4f, 5p, and 5d Subshells 155
10. Photoionization of Helium to $He^+(n=2)$: Autoionization and Final-State Symmetry 156
11. Photoelectron Angular Distributions of the N_2O Outer Valence Orbitals in the 19-31 eV Photon Energy Range 156
12. Rotationally Resolved Photoelectron Angular Distributions for H_2^+ ($v^+=0$) at λ = 584 Å and 736 Å 157
13. Rotational Relaxation in Supersonic Beams of Hydrogen by High Resolution Photoelectron Spectroscopy 157

1982 Publications and Reports 158

h. Crossed Molecular Beams
Yuan T. Lee, Investigator

1. $O(^1D)$ + HD Reactive Scattering 160
2. Photoexcitation Studies of Substituted Cycloheptatrienes 160
3. Photochemistry of Glyoxal 161
4. Elastic Scattering of ArXe and KrXe 162
5. Photodissociation of Large Water Clusters 162
6. Infrared Multiphoton Dissociation of C_2F_5CL and C_2F_5Br 162
7. Molecular Beam Studies of Vibrational Predissociation of $(C_2H_4)_2$ and $(NH_3)_2$ Using a Pulsed CO_2 Laser 163

1982 Publications and Reports 163

i. Potential Energy Surfaces for Chemical Reactions
Henry F. Schaefer III, Investigator

1. Terminal vs Bridge Bonding of Methylene to Metal Systems Al_2CH_2 as a Model System 166
2. The Weakly Exothermic Rearrangement of Methoxy Radical ($CH_3O\cdot$) to the Hydroxymethyl Radical ($CH_2OH\cdot$) 167
3. Cyclic D_{6h} Hexaazabenzene--A Relative Minimum on the N_6 Potential Energy Hypersurface 167

1982 Publications and Reports 168

3. Atomic Physics

a. Atomic Physics
Richard Marrus, Investigator

1. Parity Violation in Atoms 170
2. One Percent Measurement of the Lifetime of the $2\,^2S_{1/2}$ State of Hydrogenlike Argon (Z = 18) 170
3. Electron Capture by Low-Energy Multicharged Neon Ions 171

1982 Publications and Reports 171

4. Chemical Energy

a. Formation of Oxyacids of Sulfur from SO_2
Robert E. Connick, Investigator

1. The Rate and Mechanism of Exchange of Oxygens Between Bisulfite Ion and Water 172
2. Rates of Substitution Reactions on Metal Ions 172

1982 Publications and Reports 172

b. Catalytic Hydrogenation of CO: Catalysis on Well-Characterized Surfaces
Gabor A. Somorjai, Investigator
and
Catalysis by Supported Metals
Alexis T. Bell, Investigator

1. The Hydrogenation of CO Over Rhodium Foil, and Rhodium Compounds, $FeRhO_3$ and Na_2RhO_3 173
2. The Effects of Additives on the Fe and Re Catalyzed CO Hydrogenation Reactions 173
3. The Production of Methanol from CO and H_2 Over Thorium Oxide Catalyst Surfaces 174
4. Characterization of Carbon Deposits Formed During CO Hydrogenation Over Ruthenium 174
5. The Influence of Metal-Support Interactions on the Synthesis of Methanol Over Palladium 174

1982 Publications and Reports 174

c. Organometallic Chemistry of Coal Conversion
K. Peter Vollhardt, Investigator

1. Biscarbyne Clusters as Homogeneous Analogs of Fischer-Tropsch Intermediates on Surfaces 176
2. Transition Metal Mediated Thermal Extrusion of Sulfur Dioxide from Thiophene-1,1 Dioxides 176
3. Work in Progress 177

1982 Publications and Reports 177

d. Synthetic and Physical Chemistry
William L. Jolly, Investigator

1. An X-Ray Photoelectron Spectroscopic Study of the σ- and π-Allyl Groups 179
2. An X-Ray Photoelectron Spectroscopic Study of the Bonding in (Alkylidyne) Tricobalt Nonacarbonyl Complexes and Related Compounds 179
3. An X-Ray Photoelectron Spectroscopy Study of Transition Metal μ-Methylene Complexes and Related Compounds 179
4. Justification of the Approximation That Shifts in Nonbonding Valence Orbital Ionization Potential are Eight-Tenths of Shifts in Core Binding Energy 179
5. Work in Progress 180

1982 Publications and Reports 180

e. Chemistry and Morphology of Coal Liquefaction
Heinz Heinemann, Investigator, with Alexis T. Bell, James W. Evans, Richard H. Fish, Alan V. Levy, Eugene E. Petersen, Gabor A. Somorjai, Theodore Vermeulen, and K. Peter Vollhardt, Investigators

[See Fossil Energy Section]

f. Electrochemical Systems
John Newman, Investigator

1. Mathematical Modeling and Optimization of Liquid-Junction Photovoltaic Cells 181
2. Electrochemical Removal of Mercury from Contaminated Brine Solutions 182

1982 Publications and Reports 182

g. Surface Chemistry—Application of Coordination Principles
Earl L. Muetterties, Investigator

1982 Publications and Reports 183

h. High-Energy Oxiders and Delocalized-Electron Solids
Neil Bartlett, Investigator

1. An Electrochemically Reversible Intercalation of Graphite by Fluorine in the Presence of Hydrogen Fluoride 185
2. A Thermodynamic Threshold for the Intercalation of Graphite by Hexafluorospecies MF_6^- 186
3. Intercalation of Graphite by Silicon Tetrafluoride and Fluorine to Yield a Second-Stage Salt $C_{24}SiF_5$ 186

1982 Publications and Reports 187

i. Transition Metal Catalyzed Conversion of CO, NO, H_2, and Organic Molecules to Fuels and Petrochemicals
Robert G. Bergman, Investigator

1. Activation of C-H Bonds in Saturated Hydrocarbons on Photolysis of $(\eta^5\text{-}C_5Me_5)(PMe_3)IrH_2$. Relative Rates of Reaction of the Intermediate with Different Types of C-H Bonds, and Functionalization of the Metal-Bound Alkyl Groups 188
2. Work in Progress 189

1982 Publications and Reports 189

5. Chemical Engineering Sciences

a. High-Pressure Phase Equilibria in Hydrocarbon-Water (Brine) Systems
John M. Prausnitz, Investigator

1. Experimental High-Pressure Vapor-Liquid Equilibrium 191
2. Modeling of High-Pressure Phase Equilibria 191

1982 Publications and Reports 192

III. NUCLEAR SCIENCES
A. Low-Energy Nuclear Science
1. Heavy Element Chemistry

a. Actinide Chemistry
Norman M. Edelstein, Richard A. Andersen, Neil Bartlett, John G. Conway, Kenneth N. Raymond, Glenn T. Seaborg, Andrew Streitwieser, Jr., David H. Templeton, and Alan Zalkin, Investigators

Specific Sequestering Agents for the Actinides

1. Lipophilic Enterobactin Analogues. Terminally N-Alkylated Spermine/Spermidine Catecholcarboxamides 195
2. Ferric Ion Sequestering Agents. Selectivity of Sulfonated Poly(Catechoylamides) for Ferric Ion 196
3. Gallium and Indium Imaging Agents 197
4. Synthesis and Structural Chemistry of Tetrakis(Thiohydroxamato) Hafnium(IV) in $Hf(CH_3C_6H_4(S)N(O)CH_3)_4 \cdot C_2H_5OH$. 197

Synthetic and Structure Studies of Actinides and Other Compounds

1. Organouranium Complexes of Pyrazole and Pyrazolate. Synthesis and X-Ray Structures of $U(C_5Me_5)_2Cl_2(C_3H_4N_2)$, $U(C_5Me_5)_2Cl(C_3H_4N_2)$, and $U(C_5Me_5)(C_3H_3N_2)_2$ 198

2. Synthesis and Crystal Structures of the Tetrakis(Methyltrihydroborato) Compounds of Zirconium(IV), Thorium (IV), Uranium(IV) and Neptunium(IV) 198
3. Tertiary Phosphine Complexes of the f-Block Metals: Preparation of Pentamethylcyclopentadienyl-tertiary Phosphine Complexes of Ytterbium (II and III) and Europium (II). The Crystal Structure of $Yb(Me_5C_5)_2Cl(Me_2PCH_2PMe_2)$. 199
4. Preparation and Crystal Structure of Bis[Bis(Pentamethylcyclopentadienyl)Ytterbium(III)]un Decacarbonylferrate, $[(Me_5C_5)_2Yb]_2[Fe_3(CO)_{11}]$: A Compound with Four Isocarbonyl (Fe-CO-Yb) Interactions 200
5. Tertiary Phosphine Complexes of the f-Block Metals: Crystal Structure of $Yb[N(SiMe_3)_2]_2$ $[Me_2PCH_2CH_2PMe_2]$: Evidence for a Ytterbium-γ-Carbon Interaction 201
6. Stereochemistry of Bis(Carboxylato)Bis (Chloro)Bis(Tertiary Phosphine) Dimolybdenum Complexes; Crystal and Molecular Structure of Two Isomers of $(Me_3CCO_2)_2Cl_2(PEt_3)_2Mo_2$ 201
7. Anomalous Scattering by Praseodymium, Samarium and Gadolinium and Structures of Ethylenediaminetetraacatate Salts 202
8. Dipotassium Bis-([8]Annulene)Ytterbium(II) and Bis-([8]Annulene)-Calcium 203

Physical and Spectroscopic Properties

1. Optical Spectroscopy and Electron Paramagnetic Resonance of Pa^{4+} in $ThBr_4$ and $ThCl_4$ Crystals 203
2. Fourier Transform Spectrometry Observations of the Actinides 204

1982 Publications and Reports 205

IV. FOSSIL ENERGY

a. Electrode Surface Chemistry
Phillip N. Ross, Jr., Investigator

1. High Coverage States of Oxygen on Pt(001) and (111) 209
2. Adsorptive and Catalytic Properties of Zirconium Overlayers on Pt(001) 210
3. Adsorptive and Catalytic Properties of Polycrystalline Pt_3Ti 210

1982 Publications and Reports 211

b. Studies of Materials Erosion/Wear in Coal Conversion Systems
Alan V. Levy, Investigator

1. The High Temperature Erosion of Ductile Alloys 212
2. Methods for Characterization of Erosion by Gas-Entrained Solid Particles 212
3. Effect of Particle Velocity on the Platelet Mechanism of Erosion 213
4. Erosion of Boride Coatings 213
5. Erosion-Corrosion of Steels in a Burner Duct Test Device 214
6. Erosion of Metals in Liquid Slurries 215
7. Corrosion of Metals in Oil Shale Retorts 216

1982 Publications and Reports 216

c. Chemistry and Morphology of Coal Liquefaction
Heinz Heinemann, Investigator, with Alexis T. Bell, James W. Evans, Richard M. Fish, Alan V. Levy, Eugene E. Petersen, Gabor A. Somorjai, Theodore Vermeulen, and K. Peter Vollhardt, Investigators

Introduction 217

Task 1: Selective Synthesis of Gasoline Range Components from Synthesis Gas
A. T. Bell, Investigator, with R. Dictor and J. Canella 217

Task 2: Electron Microscope Studies
J. W. Evans, Investigator, with D. J. Coates 218

Task 3: Catalyzed Low Temperature Hydrogenation of Coal
G. A. Somorjai, Investigator, with A. Cabrera and R. Casanova 218

Task 4: Selective Hydrogenation, Hydrogenolysis, and Alkylation of Coal and Coal Related Liquids by Organometallic Systems
K. P. C. Vollhardt, Investigator 219

Task 5: Chemistry of Coal Solubilization
R. H. Fish and T. Vermeulen, Investigators, with
A. D. Thormodsen 221

Task 6: Coal Conversion Catalysts: Deactivation Studies
A. V. Levy and E. E. Petersen, Investigators, with
M. West and M. C. Smith 221

1982 Publications and Reports 222

d. Materials Characterization in Fossil Fuel Combustion Products
Donald H. Boone and Alan V. Levy, Investigators

1. Erosion of SiC Hard Coating Materials 224
2. Erosion of Ceramic Thermal Barrier Coatings 224

1982 Publications and Reports 225

e. Solution Thermodynamics of Sulfites and Sulfite Oxidation Mechanisms
Leo Brewer and Robert E. Connick, Investigators

1. The Mechanism of Oxidation Bisulfite Ion by Oxygen 226

1982 Publications and Reports 226

f. Process Chemicals Parameters in Aqueous Sulfur Dioxide Removal by Lime/Limestone Scrubbers
C. Beat Meyer and Robert E. Connick, Investigators

1. The Thermal Decomposition of Aqueous Tri- and Tetrathionate 227
2. The Structure of Dithionite Ion 227

1982 Publications and Reports 227

V. ADVANCED ISOTOPE SEPARATION TECHNOLOGY
A. Applications and Assessments of Advanced Techniques

a. Isotope Separation by Laser Photochemistry
C. Bradley Moore, Investigator

1. Determination of Arrhenius Parameters for Unimolecular Reactions of Chloroalkanes by IR Laser Pyrolysis 229

1982 Publications and Reports 230

VI. ENERGY STORAGE
Electrochemical Energy Storage
James W. Evans, Rolf H. Muller, John Newman,
Philip N. Ross, and Charles W. Tobias, Investigators

a. Surface Morphology of Metals in Electrodeposition
Charles W. Tobias, Investigator

1. Limiting Currents and the Effect of Hydrodynamic Flow on the Morphology of Zinc Deposits 231
2. Modeling of Current Distribution with Active-Passive Kinetics 232

b. Metal Couples in Nonaqueous Electrolytes
Charles W. Tobias, Investigator

1. Solubility of Potassium Salts in Selected Organic Solvents 233

c. Engineering Analysis of Electrolytic Gas Evolution
Charles W. Tobias, Investigator

1. Studies of Bubble Dynamics with the Mosaic Electrode and an Improved Data Acquisition System 234

1982 Publications and Reports 234

d. Surface Layers on Battery Materials
Rolf H. Muller, Investigator

1. Impedance and Ellipsometer Measurements of Surface Layers on Lithium 236
2. Work in Progress 236

1982 Publications and Reports 237

e. Electrode Kinetics and Electrocatalysis
Philip N. Ross, Jr., Investigator

1. Low Energy Electron Diffraction (LEED) Characterization of Metal Electrode Surfaces 238
2. Diffusion Controlled Multi-Sweep Cyclic Voltammetry for a Reversible Deposition Reaction Occurring on Rotating Disk and Stationary Electrodes 239

1982 Publications and Reports 240

f. Electrical and Electrochemical Behavior of Particulate Electrodes
James W. Evans, Investigator

1. Development and Testing of the Mathematical Model for the Hall-Héroult Cell 242
2. Work in Progress 243

1982 Publications and Reports 243

g. Electrochemical Properties of Solid Electrolytes
Lutgard C. De Jonghe, Investigator

1. Impurities and Solid Electrolyte Failure 244
2. Grain Boundaries and Solid Electrolyte Degradation 244

1982 Publications and Reports 245

h. Analysis and Simulation of Electrochemical Systems
John Newman, Investigator

1. Work in Progress 246

1982 Publications and Reports 247

VII. MAGNETIC FUSION ENERGY

a. Structural Materials and Weldments for High Field Superconducting Magnets
John W. Morris, Jr., Investigator

1. The Magneto-Mechanical Cryogenic Research Facility (MMCR) 249
2. Magnetic Field Effects on Mechanical Properties of Stainless Steels 250
3. Austenitic Fe-Mn Cryogenic Steels 250

1982 Publications and Reports 250

VIII. NUCLEAR WASTE MANAGEMENT

a. Thermodynamic Properties of Chemical Species in Nuclear Waste
Norman M. Edelstein, Investigator

1. Voltammetric Studies of the NpO_2^+ Carbonate Systems 251
2. The Solubilities of Crystalline Neodymium and Americium Trihydroxide 251
3. Hydrolysis and Hydrolytic Precipitation Reactions for NpO_2^+, Nd^{3+}, and Cm^{3+} 253

1982 Publications and Reports 254

IX. WORK FOR OTHERS
1. National Aeronautics and Space Administration (NASA)

a. Theoretical Studies of Formyl Radical Formation in Selected Combustion Reactions
William A. Lester, Jr., Investigator

1. Work in Progress 255

2. Office of Naval Research

a. Structure and Performance of Al_2O_3
Donald M. Boone and Alan V. Levy, Investigators

1. Platinum Modified Alumina Coatings 256

b. Electron-Phonon Coupling and the Properties of Thin Films and Inhomogeneous Superconductors
Vladimir Z. Kresin, Investigator

1. Systems Containing Thin Films 257
2. Josephson Tunneling and Proximity Effect 257
3. Work in Progress 258

1982 Publications and Reports 258

3. Electric Power Research Institute (EPRI)

a. Phase Equilibria for Fixed Bed Gasification Products, Byproducts, and Water
John M. Prausnitz, Investigator

1. Measurement of Phase Equilibria 259
2. Theoretical Methods for Correlation of Phase Equilibria 259

1982 Publications and Reports 260

b. Inhibitive Salts for Reducing High Temperature Oxidation and Spallation
David P. Whittle, Investigator

1. Oxidation of Ni-Cr and Co-Cr Alloys Coated with Reactive Element Salts 261

c. Investigate New Fuel Cell Electrolyte and Electrode Concepts
Philip N. Ross, Jr., Investigator

1. The Effect of $H_2PO_4^-$ Anion of the Kinetics of Oxygen Reduction on Pt 262

1982 Publications and Reports 263

d. Improved Beta-Alumina Electrolytes for Advanced Storage Batteries
Lutgard C. De Jonghe, Investigator

1. Degradation of Sodium Beta"-Alumina: Effect of Microstructure 264

1982 Publications and Reports 265

X. APPENDICES

Appendix A. Materials and Molecular Research Division Personnel

Scientific Staff 267
Support Staff 278

Appendix B. MMRD Committees 279

Appendix C. List of Seminars 281

Appendix D. Index of Investigators 287

APPENDIX VI

FY-84 Incremental Funding Requirements

Operating R&D

- Synchrotron Radiation Technology:	LBL	$ 3.9M
	SSRL	0.7M
		$ 4.6M

Programmatic Research

- Surface Science/Catalysis:	Operating	$ 1.1M
	Equipment	1.4M
- NCAM' Program Planning and Related Activities		2.0M
		$ 4.5M

Construction

- SSCL	$ 9.3M
- SSRL (SEPFF + 18° Beamline)	4.1M
	$13.4M
TOTAL	$22.5M

PLANNING STUDY FOR ADVANCED NATIONAL SYNCHROTRON-RADIATION FACILITIES

Printed March 14, 1984

The report of a study sponsored by the Department of Energy, Office of Basic Energy Sciences, and cochaired by Peter Eisenberger and Michael L. Knotek.

A new generation of synchrotron-radiation sources based on insertion devices offers gains in photon-beam brilliance as large as the gains that present-day synchrotron sources provided over conventional sources. This revolution in synchrotron capability and its impact on science and technology will be as significant as the original introduction of synchrotron radiation. This report recommends that insertion-device technology be pursued as our highest priority, both through the full development of insertion-device potential on existing machines and through the building of new facilities.

PREFACE

This report presents the results of a study by an ad hoc committee sponsored by the Department of Energy (DOE), Office of Basic Energy Sciences, with the charter to "solicit and evaluate ideas from synchrotron-radiation providers and users as to the future opportunities and technical needs for synchrotron-radiation based research." The committee was further charged "to establish from the available options a set of priorities for the timely development of both existing and new facilities that can meet those needs."

This study critically evaluates the current status and opportunities for synchrotron radiation (SR)-based science and technology, facilities, and users. The evaluation serves as the basis for a series of recommendations for SR that includes upgrading of existing facilities, new instrumentation, new facilities, and methods of increasing user participation. While the focus of the report is a series of recommended actions, it also contains data, analyses, observations, and criticisms, so that it can serve as a resource for future deliberations.

Judgement Criteria

Our judgements were based generally on the new science and technology offered by the next generation of machines and specifically on the way in which the properties of new sources lead to new experimental capabilities. Our analysis took into account the technological barriers that define the limits of SR sources and various issues affecting the use of these sources by the scientific community.

Methodology

The objective of conducting a comprehensive and critical scientific review influenced the choice of the committee members and the procedures adopted to obtain and evaluate the needed information. The committee membership of seventeen, listed at the end of this preface, was drawn from universities, industry, and DOE and Department of Defense (DOD) laboratories. These members represent a wide range of disciplines and include 12 SR users.

To further broaden the representation, we solicited the testimony and active participation of many other scientists, including the personnel of facilities involved in providing SR. The breadth and sophistication of SR-based science and technology required the participation of all these people, and we thank them for their responsiveness and assistance.

Information was first obtained at a meeting held at Sandia National Laboratories, Albuquerque on October 8 and 9, 1983. Approximately 30 speakers and 80 participants gave testimony on science opportunities, facility needs, user needs, and plans for new facilities, including the proposal for the Berkeley Advanced Light Source (ALS), which we were specifically asked to examine. Over 1000 pages of written technical information was provided to the committee, much of which has been distilled and included in this report. The meeting included special sessions for debate and criticism.

As the study proceeded, the committee issued additional calls for letters of opinion from the community and for technical and factual information necessary in our deliberations. Over a hundred such correspondences were received from a broad range of scientific, technical, and institutional interests. Their input has been evaluated, distilled, and, where appropriate, included in this report.

The committee then met in executive session three times over the next three months, at Stanford, MIT, and Exxon, to evaluate the material it had received, to reach its major conclusions concerning the priorities for SR, and to prepare the report. On November 15, 1983, in response to a request from DOE, an interim version of the major conclusions and recommendations was submitted to DOE in the form of a letter, which is included as Appendix A.

Committee Member	Institution
H. K. Birnbaum	University of Illinois
W. F. Brinkman	AT&T--Bell Laboratories
F. C. Brown	University of Illinois
M. L. Cohen	University of California-Berkeley
P. M. Eisenberger	Exxon Research & Development Company
D. E. Eastman	IBM TJ Watson Research Center
C. S. Fadley	University of Hawaii
K. H. Hodgson	Stanford University
M. L. Knotek	Sandia National Laboratories
F. W. Lytle	Boeing Company
D. E. Moncton	Brookhaven National Laboratory
D. J. Nagel	Naval Research Laboratory
J. E. Paterson	Stanford Linear Accelerator Center
E. W. Plummer	University of Pennsylvania
J. E. Rowe	University of Florida
H. G. Stever	University Research Associates
P. A. Wolff	Massachusetts Institute of Technology

CONTENTS

	Page
EXECUTIVE SUMMARY	11
Introduction	11
Recommendations and Conclusions	14
I. Existing Facilities and Projects	14
II. Major New Facilities	14
III. Alternative-Source Facilities	15
IV. Other Comments and Conclusions	15
SYNCHROTRON RADIATION	19
Introduction	19
The Physics of Synchrotron Radiation	19
Insertion Devices	20
Undulator Performance and Storage-Ring Design: The Need for Two Machines	25
Conclusions	26
SCIENCE AND TECHNOLOGY	29
Introduction	29
Experimental Opportunities for Science and Technology	29
Bulk Structure	29
Surface Structure	31
Electronic Properties: Bonding Structure and Dynamics	35
Imaging and Microstructure Fabrication	42
Emerging Techniques	48
Applications	52
Metallurgy and Materials Science	52
Phase-Transition Physics	54
Biological Structure	55
Medical Applications of SR	59
Catalysis	59
Earth Sciences	61
Plasma Physics	64
Actinide Chemistry	64
FACILITIES (USA)	67
Introduction	67
Existing Facilities	67

		Page
	National Bureau of Standards--SURF II	67
	University of Wisconsin--SRC (Synchrotron Radiation Center)	68
	Stanford University--SSRL (Stanford Synchrotron Radiation Laboratory)	68
	Cornell University--CHESS	69
	Brookhaven National Laboratory--NSLS	69
	General Summary	71
Future Facilities		72
	Brookhaven National Laboratory--NSLS Phase II	72
	Stanford University--1-GeV FEL Storage Ring	73
	Stanford University, SSRL--SSRL Enhanced Photon Flux Facility (SEPPF)	73
	Lawrence Berkeley Laboratory--1.3-GeV Advanced Light Source (ALS)	75
	Brookhaven National Laboratory--NSLS Phase III 6-GeV Facility	77
	Stanford University,SSRL--6-GeV-Ring Facility	80
	Summary of Future Facilities	83
Cost Projections for Synchrotron-Facilities Development		86
	Introduction	86
	Facility Cost Projections	87
Users		89
	Overview	89
	User Interactions	90
Research and Development		91
	Development of Science-Driven Goals	92
	R&D Activities	92
Bibliography		95
APPENDIX A	November 14, 1983 Letter to the Department of Energy	101
APPENDIX B	Survey of Synchrotron-Radiation Research Facilities Outside the USA	107
APPENDIX C	Alternate Photon Sources	117

ILLUSTRATIONS

Figure		Page
1	A Bending Magnet/Wiggler/Undulator Comparison	22
2	Spectral Brilliance as a Function of Photon Energy	23
3	The Structure of Nitrogenase	30
4	An Application of NEXAFS	33
5	Angle-Resolved-Photoemission Spectra from Ni(110)	37
6	Ion-Fragmentation Patterns for N_2 Near the Nitrogen K Absorption Edge	40
7	A Soft X-ray Microscope Utilizing a Zone-Plate Lens	45
8	Melting of a Xenon Monolayer on Graphite	56
9	An Example of K-Edge Dichromatography of the Arterial Structure of a Pig's Heart	60

TABLES

Table		
1	Undulator Performance on 1.3- and 6-GeV Machines	24
2	Six Important Methods of X-ray Imaging	44
3	Existing SR Facilities in the USA	67
4	Future SR Facilities in the USA	72
5	Experimental Beamlines and Insertions, NSLS Phase II Construction Project	73
6	PEP-Beam-Facility Design Parameters	74
7	Specifications for the PEP-Beam-Facility Undulator	75
8	ALS Design Parameters	76
9	ALS Construction Cost Estimates	76
10	Summary of Currently Planned ALS Insertion Devices (1.3 GeV)	77
11	Cost Estimates for the Construction of Booster II: NSLS Phase III	79
12	NSLS High-Energy U/W Ring Preliminary Parameters	79
13	A Comparison Between the NSLS U/W Ring and the ESRF	80

Table		Page
14	SSRL 6-GeV-Ring Parameters	81
15	Radiation Characteristics of Possible SSRL 6-GeV-Ring Sources	82
16	Storage-Ring and Device Parameters for Representative Facilities	84

EXECUTIVE SUMMARY

Introduction

Throughout the development of modern science and technology, electromagnetic radiation has been the most effective of exploratory probes for the discovery of structural characteristics and for the understanding of physical processes. Success in such discoveries has been intimately linked to evolution and revolution in the technology of photon generation. The electric light, the discharge lamp, the x-ray tube, and the laser each ushered in new eras of science. We can now add to this list the most versatile of sources: synchrotrons, or storage rings for the generation of synchrotron radiation (SR).

SR has the unique capability of providing radiation over eight decades of the electromagnetic spectrum, from 10^{-3} to 10^{5} eV. Thus, it reaches from the infrared, the visible, and the ultraviolet, through the soft and hard x-ray domains, and up to the gamma-ray region. Within the last few years we have become confident that SR facilities can be built that will provide unprecedented control of all the important characteristics of a photon beam: source size, spatial coherence, temporal coherence, spectral range, polarization, and time structure. As a source of electromagnetic radiation, only lasers and perhaps plasma sources will maintain any superiority for specific applications.

In the brief history of experimentation in the newly emerging field of SR science and scientific measurements, there are already significant accomplishments in a wide variety of fields. In solid state physics and in surface science, bulk and surface electronic structures have been measured. Grain boundaries and interfaces of important semiconductors and metals have been studied. Surface

bond lengths have been determined to a degree of resolution that is important to the study of surface chemistry. In phase-transition physics, the first studies of structural transitions in two-dimensional systems have revealed new phases and new transition mechanisms. In biology, SR has been used to define the active site in important metalloenzymes like nitrogenase, the enzyme responsible for nitrogen fixation in plants. In energy research, the concentration and chemical state of impurities in coal and the structure of bimetallic catalysts have been determined. And in medicine, a noninvasive, low-dose angiography technique with the promise of wide applicability as a general medical imaging technique has been developed. Although some of the techniques used in SR science have been used earlier with conventional photon sources, the brightness and tunability of SR has carried experiment and measurement far beyond the capabilities of the past.

Though the thrusts to date have concentrated in the basic sciences, technological applications of SR are beginning to emerge, as evidenced by recent SR studies of catalysis, medical imaging, submicron lithography for the computer industry, defect structures in solids, amorphous materials, alloy-structure determination, phase changes in solids, and applications to biological materials.

The SR field has had a similar impact in the industrialized countries of Europe and Asia. All of these countries expect the industrial and defense applications to grow rapidly in significance, and they all are building their array of SR facilities to handle the work. In some countries--West Germany, France, England, the Soviet Union, and Japan--there are SR facilities comparable to those in the USA, and these countries all have high-priority programs to advance their capabilities.

Opportunities have now been demonstrated for orders-of-magnitude improvement in SR capabilities through the use of special insertion devices called wigglers and undulators and of storage rings with improved characteristics; these innovations make it possible to enhance and optimize the radiation for specific studies. The gains are not only in the intensity of the radiation source but also in its optical qualities, which include extraordinary collimation and small source size, variable polarization, and extremely short pulse lengths. This added control will lead to experiments not previously possible.

One sees expanding horizons of experimentation in basic condensed-matter sciences, in materials science and technology, and in chemistry, biology, and medicine, in addition to increased usage of some of the past techniques with better capabilities. The added flexibility offered by higher-brilliance sources will greatly enhance the sophistication of our physical probes and make possible studies of smaller and more dilute samples and of weaker phenomena. The future offers x-ray holography, various microscopies, studies of low-energy excitations and time-dependent phenomena, the determination of the properties of very small particles, and new frontiers in atomic, molecular, and plasma studies.

To meet the challenges and opportunities in both scientific-research and technological applications of SR, facilities will be needed that are dedicated to the utilization of insertion devices and that are readily accessible to the whole spectrum of university, industry, and defense interests. New machines dedicated to the utilization of insertion devices, even if they are developed on the most expeditious schedule, will not have significant impact until the late 1980s or early 1990s. Therefore, our recommendations include the full development of existing insertion-device capability, in parallel with the construction of new facilities specifically designed for the use of these devices.

EXECUTIVE SUMMARY

Recommendations and Conclusions

I. Existing Facilities and Projects

The committee recommends that steps be taken to ensure the timely completion of the commissioning of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory and the Synchrotron Radiation Center (SRC) at Stoughton, Wisconsin. We are encouraged by the actions at NSLS and SRC since our initial letter to the Department of Energy (DOE). To optimize utilization of existing facilities, we recommend providing operations funding, so that such facilities can provide a maximum of beam time in a "user friendly" mode, and continued research funding, so that it will be possible to take full advantage of the facilities.

To realize the full potential of existing facilities, the committee recommends expeditious completion of currently approved projects to construct insertion-device beamlines: the NSLS Phase II project at Brookhaven Laboratory and the SSRL Enhanced Photon Flux Facility (SEPFF) project at the Stanford Synchrotron Radiation Laboratory (SSRL). The future construction of additional insertion-device-based beamlines at existing facilities is strongly recommended.

II. Major New Facilities

The committee believes that major new programs based on the utilization of insertion devices are of central importance for effective progress in materials-science, physics, biology, and chemistry research over the next decade. The committee is therefore unanimous in its recommendations, which follow in order of priority.

1. The design and construction of a high-energy storage ring capable of providing fundamental undulator radiation in the x-ray region of the spectrum up to 20 keV, with an early 1990s target date for full operation of the facility.

To achieve this objective, appropriate research and development funding should be allocated now.

2. The construction of a second, lower-energy ring capable of providing fundamental undulator radiation in the soft x-ray region of the spectrum up to 2.0 keV. This machine should also provide picosecond (ps) timing capabilities. The Advanced Light Source (ALS) is such a machine.

The committee strongly recommends that no action based on the second-priority recommendation interfere with the timely pursuit of the first-priority recommendation.

III. Alternative-Source Facilities

Free-electron-laser (FEL), ultraviolet (UV)-laser, and laser-heated-plasma sources promise to make important complementary contributions at the low-energy end of the spectrum. To provide a complete full-spectrum capability, these sources should be developed in as timely a fashion as possible by their respective technical communities and funding agencies. However, the committee concluded that in the foreseeable future SR will continue to be the premier source of radiation in the soft x-ray and x-ray regions.

IV. Other Comments and Conclusions

The Need for Two Machines and their Relative Priority -- The physics governing the performance of undulators dictates that a machine designed to produce x-ray radiation at energies above 10 keV operate at a different energy level than a machine designed for the optimal production of soft x-ray ultraviolet (XUV) radiation at energies less than 2 keV. Using existing or anticipated technology, fundamental undulator radiation at 10 to 20 keV will require a 5 to 6-GeV machine, while optimized undulator radiation at less than 2 keV

will require a machine operating at approximately 1.5 GeV. Factors governing the relative priority of these two machines include:

A. There are no dedicated facilities where x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.

B. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

Commissioning of New Machines -- The difficulties being experienced in the commissioning of the newly constructed machines arise from overzealous attempts at economy, from some deficiencies in the project-management systems, and from a general lack of big-project experience in the materials-science community. These are not fundamental technical problems and should be rectified in future projects.

Improving Access to Facilities -- The access to SR facilities is currently being restricted by two major factors. The first factor is the difficulty experienced by university-based groups in obtaining the funding necessary for participation. We recommend that beamline funding at future and existing facilities be provided in such a way that university-based groups can participate more readily. This cooperation would significantly broaden both the technical base that could contribute to innovations in instrumentation and the scientific base that could contribute to effective use of the facility. A proposal-based, peer-reviewed approach for the selection of outside participants is strongly recommended.

The second factor is the limitation on the participation of industry, university, and government laboratories that are performing applied research. In deciding which groups can participate

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in beamline usage, there is currently a bias towards fundamental research. The broadening of program-review committees to include applied interests, together with procedures to ensure more "user friendly" instrumentation and the protection of proprietary and classified interests, would increase the participation of applied-research groups.

Continuing Review -- The rapid developments in SR make it appropriate that a committee similar to ours convene periodically to review current developments in the entire field and to make recommendations for future actions.

SYNCHROTRON RADIATION

Introduction

Before synchrotron radiation (SR) was available for ultraviolet (UV) and x-ray experimentation, scientists relied on a collection of sources that had low intensity, lacked tunability, and in general did not provide radiation that was easily manipulated. The use of bending-magnet radiation from synchrotrons built for high-energy physics provided orders-of-magnitude increases in source intensity and brilliance and opened many research frontiers. The design of a new generation of dedicated machines (the National Synchrotron Light Source [NSLS] and the Synchrotron Radiation Center [SRC]) especially configured to produce a bright source is leading to further improvement. Now a new class of machines based not on bending-magnet radiation but on insertion devices promises increases in source brightness and quality as large as the original gains over conventional sources. It is this class of devices that has launched new initiatives for facility development. An understanding of the physics governing the performance of these new devices is necessary to appreciate the technical issues underlying the recommendations of this report. This section of the report provides the basic concepts needed for understanding the physics of insertion devices.

The Physics of Synchrotron Radiation

If the path of an ultrarelavistic electron of energy $E = \gamma mc^2$ (where m is the mass of the electron and c is the speed of light) is bent to a radius R by a magnetic field, it will emit radiation with a continuous (white) wavelength distribution centered around a critical wavelength

$$\lambda_c = R \gamma^{-3}. \quad (1)$$

The radiation is emitted into a narrow cone of opening angle

$$\delta = \gamma^{-1}. \quad (2)$$

SYNCHROTRON RADIATION

For E = 3 GeV and a typical bending radius of 20 meters, $\gamma = 6 \times 10^3$ and $\lambda = 1.0$ Å (approximately 12 keV), with an opening angle of 2×10^{-4} radians or about 40 seconds of arc. The radiation in the orbit plane is linearly polarized, and outside this plane it is elliptically polarized.

The brightness (intensity per unit solid angle and bandwidth) of such an x-ray source is 2 to 3 orders of magnitude greater than that of the characteristic lines of a modern 10-kW rotating-anode source; it is many more orders of magnitude more intense than the bremsstrahlung spectrum from such a source. Furthermore, the synchrotron source is continuously tunable, highly polarized, and directed into an extremely narrow beam. The radiation from an electron bunch comes in pulses as the electrons traverse the aperture of the beamline. For a typical single bunch, the repetition rate is on the order of hundreds of nanoseconds, and the pulse length is a small fraction of a nanosecond. This time structure has been found extremely useful in a wide variety of timing experiments. The Advanced Light Source (ALS) design would offer pulse lengths in the 10-ps range, opening a new regime for time-dependent studies.

Within the last 10 years, most SR-based experiments have been performed using whatever source characteristics the bending magnets of existing high-energy storage rings happened to have. Although the beams from these bending-magnet sources are considerably brighter than those obtained using conventional light sources, dramatic improvements are possible. The newest generation of storage rings (NSLS and SRC) has extremely small electron-beam cross section and angular divergence (i.e., low emittance), resulting in bending-magnet radiation with significantly higher source brilliance (brightness per unit source size). Even higher brilliances are possible using specially designed magnetic structures inserted in the straight sections of storage rings. The functional separation of the magnets that control the electron orbit and those that produce the radiation is an important strategic advantage allowing source design innovations to be implemented at will. The physics of these devices is described below.

Insertion Devices

A straight electron trajectory can be wiggled in a transverse magnetic field that is alternating, say N times, along the path in a device of length L. These insertion devices immediately provide an N-fold increase in intensity because the radiation from each of the N magnetic sources is superimposed in the forward direction. There are two different classes of insertion devices; the distinction between them depends on the strength of the orbit perturbation. If the electron path deviates by an angle that is approximately equal to or less than the opening angle of the SR, $1/\gamma$, then the device is called an undulator. Devices causing larger deviations are called wigglers. In addition to enhanced brillance, other characteristics of the photon beam can be controlled by varying the magnetic period $\lambda_u = L/N$ and the strength of the magnetic field B. A key parameter determining performance is $K = 0.93\ B(kG)\lambda_u(cm)$. To a first approximation, K is the ratio of the angular excursion of the electron to the synchrotron opening angle $1/\gamma$. If $K \leq 1$, the device is an undulator; for $K > 1$ it is a wiggler. The behavior of both these devices can be described by the same theory, but their properties can be significantly different. Both types have been tested and their behavior is in agreement with predictions. An N = 27, K = 8 wiggler at Stanford is currently the world's most powerful source of SR.

The total radiation produced by wigglers is similar to bending-magnet radiation in its vertical opening angle, $1/\gamma$, and its smooth spectral function. However, its horizontal opening angle is reduced to K/γ, and its intensity is multiplied by N. To understand the properties of undulators, one must take account of the interference of the radiation emitted by each of the 2N magnetic poles. This detailed interference theory is necessary as K decreases toward unity, but it is equally valid for high-K wigglers. The mathematical relationships that explain the precise properties of wigglers and undulators are contained in the footnotes below Figure 2. For the purposes of the following discussion, note that (1) undulator radiation has a structured spectrum consisting of peaks at the fundamental wavelength λ_p^1 and harmonics λ_p^m (Footnote 1), and (2) the fundamental radiation is emitted into a solid angle Ω (Footnote 2). With these definitions one can describe generally the performance of insertion devices. Figure 1 shows the spectral brilliance and the qualitative differences in the spatial character of the radiation from different sources. Spectra for two different undulators are depicted in Figure 2. Finally, Table 1 gives specific performance data for a number of different devices.

Generally, lower-K and higher-N devices (undulators) produce radiation with greater directionality. For a low-K undulator, the solid angle $\Omega = \frac{1}{\gamma^2 N}$, and it contains a quasi-monochromatic beam with a fractional bandwidth $\Delta\lambda/\lambda$ equal to $1/N$. The total number of photons in this beam is increased by a factor of N and the brightness by a factor of N^2, compared with a beam from a bending magnet. Typically, $N = 100$, so the gains are substantial. As shown by Footnote 4, the power in the fundamental P_1 is a substantial fraction (two thirds) of the total device power P_{TOT} when $K = 1$, and $P_1/P_{TOT} \to 1$ as $K \to 0$. Therefore, the most efficient production of radiation in a narrow bandwidth around λ_p occurs for devices with $K \lesssim 1$. As K increases with fixed λ_p and L (by varying either λ_u or γ), the solid angle Ω remains constant. Thus, a high-K device is still capable of producing highly directional radiation of wavelength λ_p with N-fold intensity enhancement. However, this solid angle now includes substantial higher-harmonic power given by $\frac{K^2}{2} P_1$, and the bandwidth is increased to $(1 + K^2/2)/N$. This decrease in coherence is a direct result of the large angular excursions of the electron in a high-K device, which diminish the relative range of angles over which constructive interference occurs.

Before discussing the specific consequences of the behavior described above for the next generation of machines, one more point should be made. The brilliance of $K = 1$ undulator beams is potentially so high that their ultimate quality is strongly dependent on the emittance of the storage ring. First, the spatial size of the electron beam in a storage ring must be small enough so that at a reasonable distance d one can select out an area $d^2\Omega$ through which the first harmonic will pass. Second, the angular divergence of the electron beam should be on the order of $\Omega^{1/2}$ or smaller. For this reason, the next generation of storage ring will be designed with very low emittance.

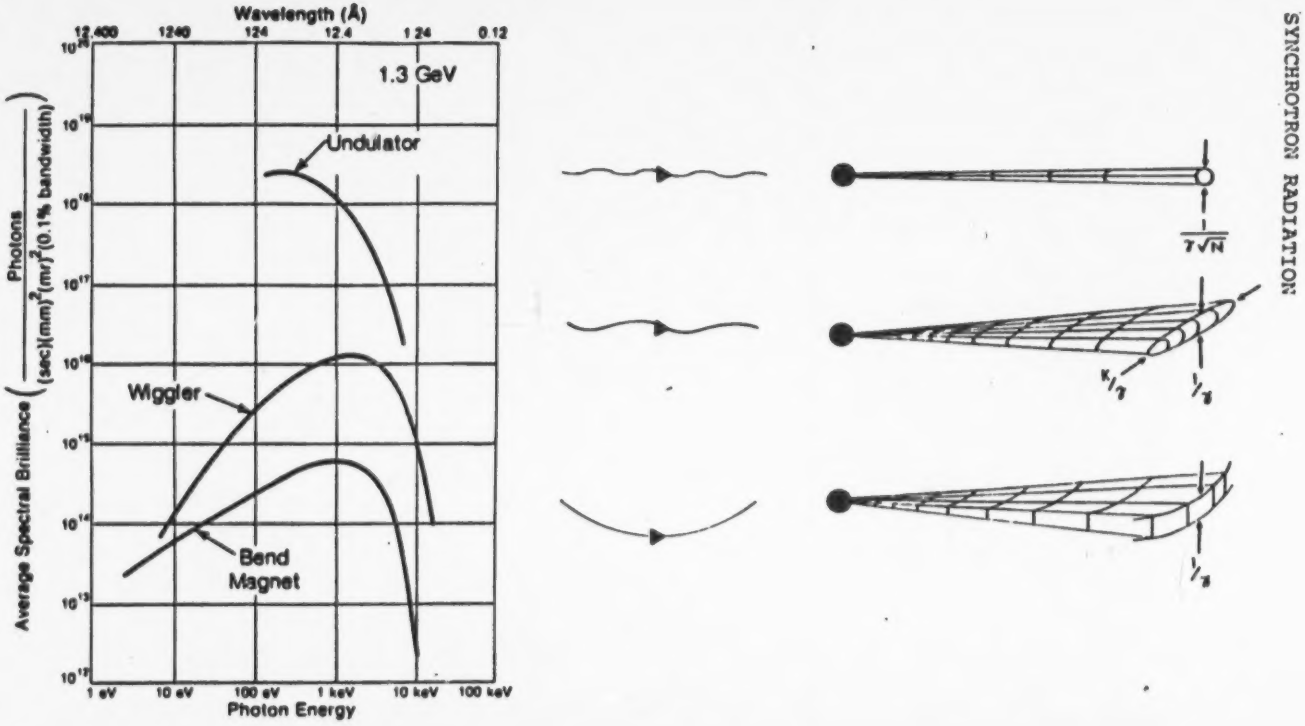

Figure 1. A Bending Magnet/Wiggler/Undulator Comparison. Left: The spectral brilliance as a function of photon energy for a bending magnet, wiggler, and undulator on a 1.3-GeV ring (the ALS design). The undulator curve is actually an envelope; the detailed spectral dependence is shown in Figure 2. Right: The approximate relationship between the electron-beam oscillations for the bending magnet (bottom), wiggler (middle), and undulator (top), and the respective angular distributions of their radiation. Undulator radiation is emitted in an intense laser-like beam.

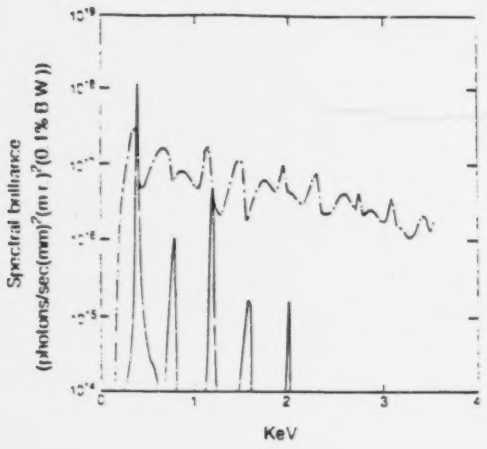

Figure 2. Spectral Brilliance as a Function of Photon Energy. Spectral brilliance through a pinhole aperture as a function of photon energy is shown for the 400-eV-fundamental-energy undulators of Table 1, for both the 1.3-GeV ring (solid line) and the 6-GeV ring (dashed line). The spectral brilliance and purity of the 1.3-GeV machine is diminished at 6 GeV, while the power to the optical element is increased.

Footnotes: Insertion-Device Properties

The fundamental wavelength λ_p of an undulator of period λ_u at an opening angle σ is:

$$\lambda_p^m = \frac{\lambda_u}{2\gamma^2 m}\left(1 + K^2/2 + \gamma^2\sigma^2\right) \qquad \text{(FN1)}$$

The radiation is emitted into an opening angle

$$\Omega = \left(1 + \frac{K^2}{2}\right)\frac{1}{N\gamma^2} = \frac{2\lambda_p}{L} \qquad \text{(FN2)}$$

The power in the fundamental is:

$$P\left(\lambda_p\right) \propto \frac{K^2 N}{1+K^2/2} \qquad \text{(FN3)}$$

The ratio of the total power to the power in the fundamental is:

$$\frac{\Sigma_m P_m}{P_1} = 1 + K^2/2 \qquad \text{(FN4)}$$

The total power from the device is:

$$P_T = 0.127\ (E(GeV))^2 \langle B(kG)\rangle^2\ L(cm)\ I(A) \qquad \text{(FN5)}$$

Table 1

Undulator Performance on 1.3- and 6-GeV Machines

Conditions: The total power is constant in the comparison between the 1.3- and the 6-GeV rings at any energy, assuming that E^2B^2L is constant. That is, the beam current is fixed (at 400 mA) in the comparison.

Machine Energy (GeV)	E_1 (eV)	λ_u (cm)	B_o (T)	K	N	Total Power (W)	Power Density at 10 m (W/mm^2)	Power in the Central Spot (W)	Brilliance (photons/s-mm^2-mrad^2-0.1%BW)
1.3	100	10	0.12	1.1	50	30	0.7	1.6	3.2×10^{17}
6	100	95.5	0.0255	2.27	5	30	7	16	4.9×10^{16}
1.3	200	5	0.236	1.1	100	120	3.0	4.5	1.3×10^{18}
6	200	47.7	0.051 .057	2.27	10	120	29	43.5	1.9×10^{17}
1.3	400	3.5	0.165	0.54	142	58	3.00	3	1.2×10^{18}
6	400	42.5	0.035	1.42	12	60	24	24	3.1×10^{17}
6	15,000	2.15	0.176	0.346 .351	230	1400	1700	850	4×10^{18}

Undulator Performance and Storage-Ring Design: The Need for Two Machines

Footnote 1 provides the basis for choosing the energy E of the machine necessary to produce a K = 1 device operating in the range 0.5 A < λ_p < 1.0 A. For a fixed-length straight section, it is best to make the period λ_u as small as possible for K = 1. The limit on λ_u is determined by magnet technology and results in a machine-energy requirement of 6 GeV. There is a similar optimum energy of about 1.5 GeV for producing fundamental undulator radiation with λ_p > 10 A. Nevertheless, there is a basic asymmetry between the two machines: A high-energy machine can produce lower-energy undulator radiation by making λ_u or K larger, but a low-energy machine cannot produce first-harmonic radiation in the x-ray region because of the lower limit on λ_u. To use higher harmonics for this purpose requires large K and greatly diminished brilliance. Let us consider in more detail two important technical issues relevant to our recommendations: (1) the problems of producing soft x-ray ultraviolet (XUV) (λ_p < 10 A) undulator radiation on a 6-GeV machine and (2) the thermal loads generated by hard-x-ray undulators on a 6-GeV machine.

(1) To produce λp = 10 A with E = 6 GeV requires a reduction in N (an increase in λ_u, for fixed L) and changes in either K or B or both. Table 1 compares XUV devices on the ALS machine with devices to produce the same λ_p on a 6-GeV machine. In this comparison K and B are changed in the device in such a way as to keep constant the total power produced. The result for the 400-eV device, for example, is a reduction in brilliance on the 6-GeV machine by a factor of four and a concomitant increase in the power in the central spot by a factor of eight. Clearly, the beam quality has diminished. Also, the power densities may exceed those tolerable on delicate XUV monochromators. In addition, the spectral purity is decreased, as shown in Figure 2.

(2) The power densities produced by hard x-ray undulators are clearly high, as demonstrated by the last entry on Table 1. This issue will be the subject of substantial research and development during the preparation of proposals for 6-GeV facilities. It is, however, already clear that the total power and power density can be withstood by properly engineered nonoptical components. This conclusion follows from considering the powers and power densities created in fixed-target x-ray tubes (~ 1/2 kW/mm^2). Starting from the power density of 2300 W/mm^2 at 10 meters that is listed in Table 1, adjustments should be made for the placement of components at larger distances from the source and and for the implementation of oblique-incidence geometries. Furthermore, for purposes of the comparison in Table 1, the same currents were used for both machines. It is unlikely that a 6-GeV machine would have such a high current. The combination of all these factors diminishes the expected power densities to a few tens of W/mm^2, well below known thermal limits for nonoptical components. Further research and development will be necessary to develop thermally robust optical components, but the situation is clearly less critical than for XUV optics.

To use a 6-GeV ring for soft-x-ray science, the higher-order power from the beam must be removed before the beam strikes the first focusing optical element. There exists in principle a solution to the higher-order-power problem, using

total-external-reflection optics. The basic concept is that by properly chosing the mirror material and the angle of reflection, the unwanted high-energy photons can be absorbed on the first metal mirror. This is common practice in the hard x-ray region. For the XUV region, an aluminum mirror at 30-mrad incident angle would absorb the higher harmonics well at energies between 800 and 1000 eV. A fundamental difference between work in the XUV and the x-ray regions is that experiments in the XUV commonly span up to two decades in energy (e.g., 20 eV to 2000 eV), while in the x-ray they rarely span a factor of two. Utilizing the total-external-reflection phenomenon in the XUV region is thus much more complicated because for every factor-of-two energy range, a separate mirror is needed. Use of the total-external-reflection phenomenon in the XUV will be further complicated by carbon contamination of the mirror, which is more of a problem in the XUV and which occurs at a higher rate on a 6-GeV ring. Research and development will be needed to determine the extent to which utilizing the total-external-reflection phenomenon can make a high-energy ring useful in the XUV region. While the above problems can be extreme on a new 6-GeV ring, they are much reduced on a 2.5-GeV machine like the NSLS.

In addition to the power-handling problem, the time structure of a 6-GeV machine will be worse than that of an ideally designed small ring by a factor of two to five. In principle, short pulses could be attained with a 6-GeV ring; this is accomplished with lattice changes and optics and rf-driver modifications that are more complex and expensive on a 6-GeV ring than on a 1.3-GeV ring. The cost of UV beamlines will also be higher on a 6-GeV ring, due to the scaling in size and the more complex optics.

Conclusions

Given these considerations, the need for separate machines optimized in the hard and soft x-ray regions, respectively, becomes apparent. In determining the relative priority of the two machines, there are two factors to be considered.

1. There are no dedicated facilities where hard x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.

Of the two high-energy (E > 4 GeV) storage rings operating in the USA (PEP and CESR), neither has any prospect of dedicated operation. Nevertheless, important experience could be gained by developing undulators for research-and-development purposes on these rings. Such a device is now part of the SSRL (Stanford Synchrotron Radiation Laboratory) Enhanced Photon Flux Facility (SEPFF) construction project.

On existing dedicated lower-energy rings (the SPEAR, Aladdin, and NSLS rings), undulators to serve the XUV regime are now under design or construction. Because other undeveloped straight sections exist at these facilities, new construction could be undertaken to further increase the XUV capacity.

2. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

The production of x-rays on a low-energy ring is limited to the use of high-field wigglers. Although these sources do not represent an improvement in flux over beams produced by bending magnets on SPEAR and at NSLS, they would represent an increase in capacity.

Soft x-ray undulator radiation produced on a high-energy machine would have a brilliance that is lower than that produced on an optimal lower-energy machine but higher than that produced by existing devices. Therefore, in principle, the high-energy machine could provide new XUV capability. However, two substantial difficulties arise. First, the spectral purity is compromised, and second, the power in the central spot may exceed the power-handling limits of current optical technology.

SCIENCE AND TECHNOLOGY

Introduction

The properties of insertion devices as sources of radiation are clearly impressive, yet our recommendations must ultimately have a scientific foundation. In our deliberations, the scientific case presented in this section gradually emerged. While not exhaustive, the range of topics presented here does reflect the cross-disciplinary breadth of synchrotron radiation (SR) research.

This section presents brief descriptions of individual research topics, descriptions that are divided into the general areas of techniques and applications. The bulk-structure, surface-structure, and electronic-properties sections discuss general capabilities, accomplishments, and future opportunities offered by enhanced brilliance. Sections on imaging techniques and emerging techniques discuss substantially new approaches made possible by new capability. The applications sections present more specific examples of the types of fundamental and technological problems to which SR can be applied. These examples show that while SR research has a strong fundamental character, it also has a growing relevance to technology.

Experimental Opportunities for Science and Technology

Bulk Structure

X-ray-Absorption Spectroscopy (EXAFS and NEXAFS) -- The extended x-ray-absorption fine structure (EXAFS) technique is among the most widely used and mature of SR methods for determining local structure, and it is the method of choice for structural investigations in certain disciplines. Important results have been obtained in the fields of catalysis, biology, metallurgy and materials science, and surface science, to name just a few.

EXAFS specifically deals with fine structure at $E > 50$ eV above an absorption threshold. In addition, analysis of near-edge x-ray-absorption fine structure (NEXAFS)--also referred to as XANES (x-ray-absorption near-edge structure)--for $E < 50$ eV above an absorption threshold, can provide comple-

mentary information on local electronic and atomic structure and has found equally broad applications.

EXAFS and NEXAFS are discussed in detail in the following sections that deal with the different individual areas of study in which they have been applied. Particularly important examples of the application of these techniques are found in the sections on biology, metallurgy, micromineralogy, catalysis, and surface structure. An example of their application to biology is the determination of the structure of the active site for nitrogen fixation in nitrogenase. The structure of nitrogenase is illustrated in Figure 3.

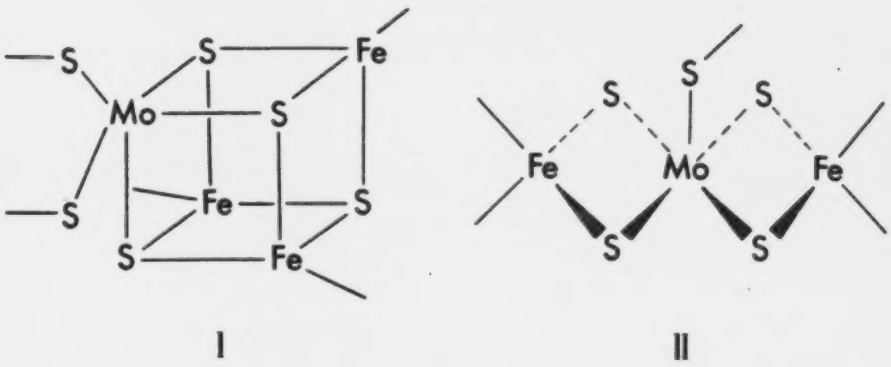

Figure 3. The Structure of Nitrogenase. The enzyme nitrogenase is responsible for the conversion of atmospheric dinitrogen into amonia, which can be assimilated by growing plants. The structural aspects of the molybdenum site in nitrogenase, where this conversion reaction is carried out, were elucidated for the first time by EXAFS, thus stimulating activity toward synthesis of inorganic analogues.

Bulk Crystallography -- Crystallographic research carried out in the past few years at synchrotron x-ray sources has led to significant advances in a number of areas, notably including the study of anomalous dispersion and of diffraction from very small single-crystal samples. In addition to measuring large anomalous-scattering effects near absorption edges and demonstrating the enormous power of methods of crystal-structure determination utilizing the tunability of synchrotron sources, recent studies are uncovering fascinating dichroic effects associated with "white line" resonant absorptions. X-ray-diffraction data have now been obtained from crystals less than 20 μm in diameter, thus opening up the possibility of structural analysis of a wide variety of technologically-important substances such as zeolite molecular sieves. Areas of crystallographic research with SR that are still largely unexplored but that offer great promise include the determination of electron-density distributions in solids (using ultra-high-resolution diffraction data) and the study of time-dependent structural effects, e.g., the response of materials to pertur-

bations such as laser excitations or varying electric fields. These time-resolved applications will require advanced high-speed parallel data-collection systems with position-sensitive detectors.

Some very significant advances may be expected in many areas of powder diffraction because of the improved resolution available with SR. For example, it will be possible to apply the Rietveld technique, which involves fitting the complete diffraction profile to some structural model, to the analysis of considerably more complex structures having perhaps as many as 100 to 200 parameters and also to the study of phase transitions in which there is a very small distortion of the structure. Other important applications of SR are to peak-shape analysis for particle size, strain broadening, disorder, and thermal diffuse-scattering effects; to search-and-match techniques; and to the indexing of unknowns. Anomalous-scattering methods will be very useful in powder studies, in order to contrast specific elements, especially when they are present in low concentrations in multiphase systems such as supported catalysts.

Surface Structure

A crucial problem in the study of solid surfaces is the determination of atomic positions or bonding geometries for species within the first few atomic layers. Atomic-structure information is essential to understanding the basic physics responsible for the surface structure and the properties of that surface (such as chemical reactivity). Historically, the most useful surface-structure information has come from the "surface sensitive" probes: electrons, ions, and neutral atoms. However, with the advent of SR, the photon has emerged as the most versatile of probes. Photon-based surface-structure techniques can be surface sensitive under some circumstances and highly penetrating under others. In the case of x-ray diffraction, crystallography techniques, which have routinely yielded the atomic structures of most known bulk crystals, are now being used to determine surface structures. When local-structure information is desired, spectroscopy techniques such as surface extended x-ray-absorption fine structure (SEXAFS), NEXAFS, and photoelectron diffraction have been applied with great success. The following sections discuss each of these techniques in more detail.

SEXAFS -- The SEXAFS technique applies the concepts of the established (bulk) EXAFS technique to the determination of atomic arrangements at surfaces. Like EXAFS, the SEXAFS technique measures the x-ray absorption coefficient of an atom that is selected by its absorption edge. The detailed modulations of the x-ray-absorption coefficient, which are caused by the scattering and interference phenomena of the excited photoelectron wave, are used to probe the local environment of a selected atomic species in the surface complex. Measurement of the x-ray-absorption coefficient is accomplished in a surface-sensitive mode, usually by means of total-electron-yield or Auger-electron-yield detection. Fourier transformation of the measured modulations yields very accurate (± 0.01 Å) measurements of the lengths of the bonds between the selected surface atom and its neighbors, as well as its coordination number. These positional accuracies are 5 times higher than those of the electron-diffraction methods that were previously used and developed. The power of SEXAFS lies not only in its accuracy but also in its applicability to disordered surface complexes whose local structure could not previously be resolved.

SCIENCE AND TECHNOLOGY

Since the beginning of SEXAFS spectroscopy in 1978, the technique has been developed into a reliable surface-structure tool. About 30 surface-structure determinations have been successfully carried out so far, including the determination of the structure of atoms and molecules bound to metal and semiconductor surfaces and the determination of the growth of metal/semiconductor interfaces. The technique now has a sensitivity of about 1/3 of an atomic surface layer. Next-generation x-ray and soft x-ray sources will permit sensitivity increases of 100 to 1000 times and will make it possible to carry out experiments much more rapidly, in order to observe time-dependent dynamic effects. With increased brightness of the x-ray source, it will also be possible to develop a microscope based on SEXAFS than can be used to study the structure of surface regions approximately 1 μm in size.

NEXAFS -- A technique related to SEXAFS is NEXAFS, also referred to as XANES. NEXAFS involves the modulations of the x-ray-absorption coefficient within about 50 eV of the excitation threshold. This energy region, which is usually ignored in the SEXAFS analysis, provides important structural information that in many cases is complementary to the information obtained through SEXAFS. It is this region that exhibits the largest modulations of the absorption coefficient and that is therefore the most easily recorded experimentally. The theoretical interpretation of the near-edge structures was first tested on gas-phase molecules and recently has been applied to chemisorbed species, like hydrocarbons on transition-metal surfaces. NEXAFS makes it possible to use a technique that is sensitive to molecular structure to monitor chemical-reaction processes of molecules on surfaces. NEXAFS readily reveals the molecular orientation, the hybridization of the intramolecular bonds and the intramolecular-bond lengths. The importance of such information lies in the elucidation of the catalytic-reaction paths of molecules on surfaces. The sensitivity of NEXAFS is now about 1/10 of an atomic surface layer. Again, improved x-ray sources will greatly increase the sensitivity. More importantly, because of the large size of the modulations and the relatively small energy range (50 eV) needed for NEXAFS studies, it appears that it will be possible to record a complete NEXAFS spectrum in a short time interval and thus record time-dependent phenomena.

Surface Crystallography -- Developments in this field demonstrate the potential for making surface-structure determination as routine as conventional crystallography. The variety of systems amenable to study is large because the high synchrotron flux provides reasonable signals even from low-Z materials and because the penetration depth allows studies of deep layers and interfaces. Contrast with the substrate or the bulk can be achieved naturally (if the adsorbate or reconstructed structure is incommensurate), by employing anomalous scattering techniques with the absorbate atom of interest, or by using an adsorbate to "decorate" a reconstructed surface. The penetration depth can be varied from the bulk absorption length in normal incidence to the extinction length in a total-external-reflection geometry.

Surface reconstruction is one of the most interesting of surface-structure problems. So far, experimental work has been carried out on the reconstruction of the (100) surface of germanium, and plans are underway for studies of the 7 x 7 structure of silicon. Preliminary studies of the Au(110) surface have demonstrated that in very favorable cases, high-intensity rotating-anode x-ray sources provide enough flux. However, it is clear that the wider possibilities using synchrotron sources will eventually include much more ambitious structural

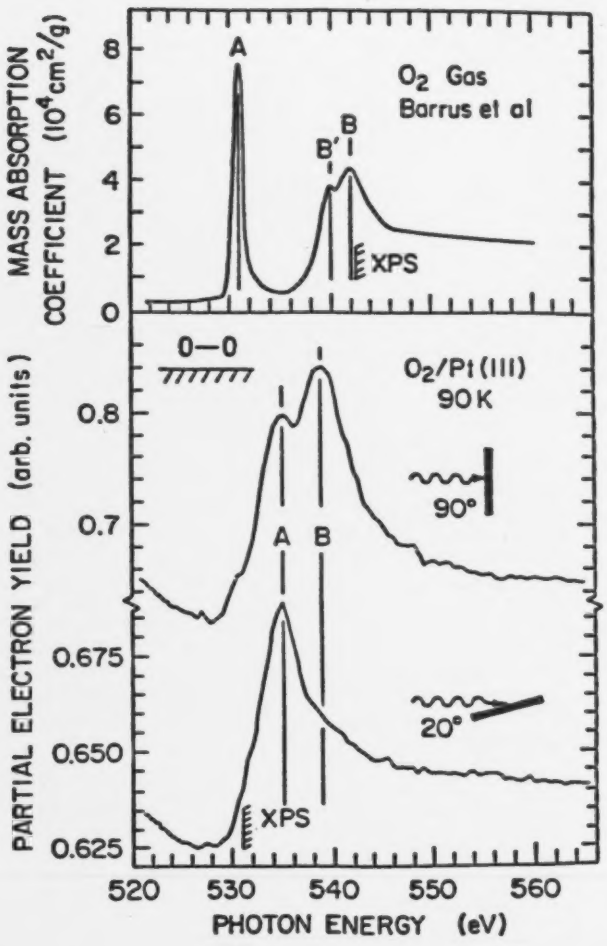

Figure 4. An Application of NEXAFS. This figure provides an example of the use of the NEXAFS technique to determine the orientation of an adsorbed molecular species, O_2 on Pt, utilizing the sensitivity of the π and σ resonances (A and B, respectively) to the polarization of the photon beam. The measurement determined not only that the oxygen was molecular on the surface, but it also determined the orientation of the oxygen and the O-O bond length.

work involving more complex systems and smaller atomic motions. In the latter category is work on the reconstructed surfaces of transition metals such as tungsten and molybdenum. Another category of reconstructed surfaces involves insulators, about which very little is known because they cannot be studied with electron techniques.

Adsorbate systems have received substantial attention so far, perhaps because the surface preparation involved is often simpler than for reconstructed surfaces. Studies of lead monolayers on single-crystal copper have revealed a metastable commensurate structure and a stable one-dimensional incommensurate structure and have documented the melting process at high temperatures. A variety of experimental studies of adsorbates (Xe, Kr, O_2, CF_4, Ar, N_2) on various graphite substrates, including single crystals, have been conducted. Important issues include incommensurability, orientational epitaxy, and the nature of various phase transitions (see the later section, "Phase-Transition Physics").

A number of studies of thin films have been carried out in two principal categories, amorphous films (studied by anomalous scattering) and freely suspended liquid-crystal films. This work has revealed a number of exciting physics and materials-science issues and promises to be a very active area as synchrotron beamlines become more generally available. X-ray beams that are more intense and more highly collimated would make possible a host of improvements in these studies: (1) extension to a wider variety of systems, (2) increased resolution, (3) the development of diffraction microscopy, and (4) time dependent studies, such as was pioneered recently in work on Si and Ge recrystallization following laser annealing.

Photoelectron Diffraction -- In this technique, as in SEXAFS/NEXAFS, core-level excitations are involved, but the emitted-photoelectron intensity is measured in a specific direction. Diffraction associated with photoelectron scattering from various atoms near the emitter produces modulations in intensity as a function of either the emission direction or the incident-photon energy. Changing the photon energy changes the diffraction by altering the electron wavelength, as in SEXAFS.

Such measurements are found to be very sensitive to the type of surface bonding site involved and have also been shown to be capable of determining adsorbate positions to within approximately 0.05 to 0.01 A. Although such measurements have been carried out over photoelectron energies from approximately 30 to 1500 eV, working at energies greater than 200 eV results in a single-scattering process similar to that used in SEXAFS. Applying Fourier-transform methods to data obtained by scanning the photon energy may yield bond distances very directly. In addition, at energies greater than 1000 eV, simple forward-scattering from nearest-neighbor atoms can produce peaks in intensity along bond directions, thus providing very direct structural information.

Systems studied so far have included atomic and molecular adsorbates on metals and semiconductors, metal/semiconductor interfaces, and layered compounds. Adsorption on stepped surfaces used as models for catalysts has also been studied. Thus, a wide range of problems is accessible with this technique.

In studies of very dilute surface species, the high intensity and tunability of SR is crucial for future work. However, the lack of SR sources in the

difficult region of 500 to 1500 eV has led to a considerable number of high-energy studies being performed with standard x-ray sources. Using these sources, angle scans may take several hours, so it is clear that next-generation SR sources planned for this energy regime will much facilitate photoelectron diffraction. In addition, the directional selectivity required in the diffraction measurement reduces intensities by a factor of approximately 100 below those in SEXAFS, so that higher-intensity sources are needed over the full spectral range from 100 to 1500 eV. Having a much-higher energy resolution of approximately 0.1 eV would also permit separate study of the diffraction effects associated with different chemically-shifted core peaks; for example, diffraction from first-layer and second-layer atoms could be distinguished for certain surfaces. Finally, a very finely focused photon beam should permit such measurements with a spatial resolution of 20 μm or less.

Electronic Properties: Bonding Structure and Dynamics

Photoemission from Solids and Solid Surfaces — Photoemission refers to the measurement of the energy distribution of electrons emitted when a photon is absorbed by matter of any form. Photoelectron spectroscopy has always been a very useful tool for probing the electronic states of atoms, molecules, and solids, but the use of SR sources in the last 10 years has revolutionized this field.

1. Angle-Resolved Photoemission

Angle-resolved photoemission has become to electronic structure what x-ray scattering is to crystallography and neutron scattering is to phonon structure. In general, given a single crystal, the three-dimensional bulk or the two-dimensional surface band structure can be determined. The unique capabilities that are available with a polarized, tunable, and intense radiation source allow the experimenter to tune to any part of the two- or three-dimensional band structure and to determine the orbital symmetry of each state. These simple symmetry rules have been used to determine bulk band symmetries, surface state (intrinsic or extrinsic) orbital character, and the bonding orientation of adsorbed molecules. Electronic-structure measurements have been made on such materials as simple metals or semiconductors, transition metals and rare-earths, compound semiconductors and alloys, and intercalated graphite and layered compounds.

Angle-resolved-photoemission measurements on surfaces of single crystals have revealed in detail the character of the two-dimensional states for clean surfaces, i.e., surfaces with atoms or molecules adsorbed from the gas phase or with bulk impurities segregated to the surface. Not only can the electronic states of the adsorbate/substrate bond be observed, but the adsorbate/adsorbate interaction can also be measured, either directly or through the substrate.

2. Core-Level Spectroscopy

There is a type of photoelectron spectroscopy that is conceptually different from the type described above; it involves removing electrons from core levels instead of from the valence or conduction bands. This type of experiment, which is called ESCA (electron spectroscopy for chemical analysis), measures the binding energy of core levels as a function of the bonding configuration

of the atom. The binding energy depends upon the surroundings of the atom being studied, such as the coordination number and the charge transfer. For example, the 4f core level of Ta will shift approximately 0.4 eV for a surface atom compared to the bulk atom, and adsorption of oxygen will cause a chemical shift of approximately 1 to 2 eV. The inherent line width of these 4f states is approximately 0.1 to 0.3 eV.

The advantages of SR for these core-level studies lie in the energy resolution, tunability, and intensity. A resolution of 0.1 eV is available from up-to-date grating monochromators. The tunability of the synchrotron makes it possible to either optimize the cross section or to select a kinetic-energy regime to accentuate the bulk or surface contribution to the spectra. This form of high-resolution ESCA has been used successfully to observe such phenomena as the various oxide states of a surface such as Si; the difference in surface chemistry on terrace or step sites; the shift in core levels at the clean surface compared to that in the bulk; the shift induced by chemisorption of a foreign atom or molecule; and the charge transfer in intercalated graphite.

An example will clearly demonstrate the impact of synchrotron core-level spectroscopy. On a Pt(111) crystal there is a 0.32-eV reduction in the $4f^{7/2}$ binding energy of a surface atom compared to that of a bulk atom, but a Pt atom at a step edge on the surface experiences a 0.58-eV reduction in binding energy. Once the step atoms were identified, the experiments showed that CO adsorbed onto a surface with steps bound preferentially to the Pt atoms at a step, thus causing the binding energy of the Pt atom to increase by 1.29 eV (0.7 eV higher than the binding energy of a bulk atom). This observation was expected, due to charge transfer from the Pt d-states into the CO 2π level during the process of bonding. In contrast, this study showed clearly that the addition of K as a catalytic promoter did not donate electrons to the Pt d-states as all models had predicted, thus suggesting that the simple models for alkali promotors must be reevaluated.

3. The Future with Insertion-Device Machines

For most problems, angle-resolved photoemission can be accomplished with the intensity and resolution available with the current-generation bending-magnet machines. However, there are several modifications of the conventional experiment that require considerably more brightness. In contrast to angle-resolved photoemission, high-resolution core-level spectroscopy can benefit immensely from the new-generation insertion-device machine.

The ultimate angle-resolved-photoemission experiment should resolve not only the energy and momentum of the emitted electron but also the spin polarization. The limitation is the 10^{-3} to 10^{-6} efficiency of spin-polarization detectors. Given the capability to resolve spin polarization, the detailed character of the exchange splitting and the spin polarization as a function of temperature could be determined for any point in the two- or three-dimensional band structure; phase transitions in rare-earth intermetallic compounds could be investigated; current theories of itinerant ferromagnetics could be tested; and magnetic properties of surfaces could be investigated.

A study of magnetic surface properties has recently been carried out in Europe. Figure 5 shows angle-resolved-photoemission spectra from a specific point in the surface Brillouin zone of Ni(110). The two peaks near the Fermi

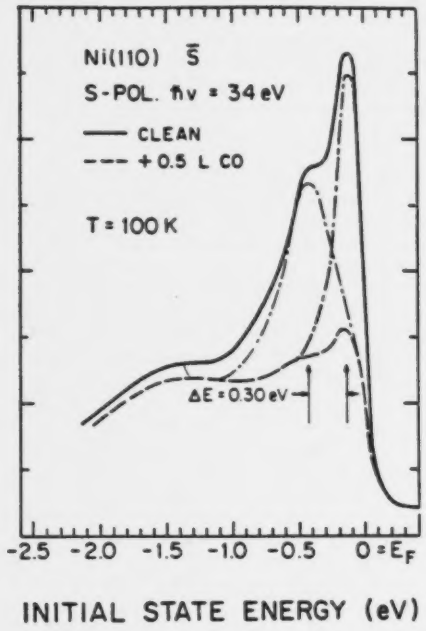

Figure 5. Angle-Resolved-Photoemission Spectra from Ni(110)

energy are surface states, one from the majority spin band and the other from the minority band. The exchange splitting is 0.3 eV, approximately equal to the bulk exchange splitting of Ni. This measurement clearly shows that the surface of Ni is not magnetically "dead." Future work will measure the net macroscopic polarization in each state as a function of crystal temperature. The local exchange splitting will persist above the Curie temperature, but the polarization will disappear. Such an experiment would lead to an understanding of the surface magnetization, including both the surface Curie temperature and the magnetic domain size. Eventually one wants to study the magnetic properties of surfaces that are contaminated with impurities.

Clearly, undulators would make spin-polarized experiments as easy as angle-resolved photoemission is today. It is important to be able to tune the incident polarization; such control could be achieved by means of a combined vertical and horizontal undulator. The momentun resolution of most energy analyzers now used at synchrotron facilities is too large for studies at higher photon energies or for samples with large unit cells. A reduction of an order of magnitude or more in signal will result when the momentum resolution is improved. The new high-brightness insertion devices will allow measurements to be routinely conducted with better energy and angular resolution.

Modern grating monochromators specially adapted to the unique source characteristics of a storage ring promise to give a resolution of better than 0.1 eV (up to 1000 eV). To estimate the flux available at this resolution, it can be noted that a typical commercial ESCA instrument using an Al target at 1 kW delivers approximately 10^{12} photons/s/30 mm^2. The inherent resolution due to the $Al_{K\alpha}$ line width is 0.83 eV. When the resolution is improved to approximately 0.3 eV by using any of the commerical 0.5-meter quartz-crystal monochromators, the counting rate is reduced by approximately two orders of magnitude. In contrast, a new toroidal grating monochromator will conservatively yield 4.0×10^{10} photons/s/mm^2 at 0.3 eV resolution when coupled to a bending magnetic with a 0.5-A beam current. This performance is an improvement over that available with commerical ESCA instruments, but it is probably not significant enough to bring a large majority of conventional ESCA users out of their laboratories.

The performance is considerably better using an undulator on a machine operating at approximately 1 GeV. A good monochromator could produce in excess of 10^{12} photons/s/mm^2 with a resolution of 0.1 eV. Compared to what is available with conventional ESCA instruments, this performance represents an increase in flux of at least two orders of magnitude and an order-of-magnitude improvement in resolution. Such a capability would allow the study of very small concentrations and dynamical processes. For example, it is quite possible that the thermal evolution of any species such as an adsorbate, impurity, or intercalant could be followed directly.

4. Excitation Experiments

The order-of-magnitude increase in brightness available from undulators will make it quite feasible to measure the angle-resolved-photoemission spectra of normally unoccupied states that have been populated by laser excitation. The few experiments that have been attempted in this area indicate that excitation is accompanied by quite dramatic charge redistribution in the occupied bands.

There are many coincidence-type experiments that become possible with the increased signal available from an insertion device. In many of these experiments, one of the channels is the energy-resolved electron that is emitted either by the direct ionization or by the subsequent Auger decay. The sections in this report on gas-phase spectroscopy and photon-stimulated desorption discuss experiments in which one of the coincidence channels is the ion fragment and the other is the emitted electron. There is also a class of experiments that is concerned with electron/electron coicidence between the primary emission and the subsequent Auger decay. For example, one channel could be set on the surface core-level peak for a step-edge atom, and the other channel could sweep through the Auger signal. This technique would give direct information about the local density of states on an atom located at a step.

Gas-Phase Spectroscopy

1. Current Studies

Gas-phase spectroscopy as practiced at SR facilities is primarily the study of highly excited states of atoms and molecules. This study includes the characterization of the electronic states of these many-particle systems, of the decay channels of the excited states, and of the interaction of the excited

atoms or molecules with other gas-phase molecules. In the last decade, the scientific progress in this small but active area of research has been substantial, and the new generation of insertion devices will lead to revolutionary improvements.

Experimental investigations of the resonance states (shape resonances) in the continuum of molecules, coupled with theoretical calculations, have lead to a clear understanding of the origin of shape resonances. The symmetry properties of these resonances are now commonly used to determine the bonding orientation of molecules adsorbed on surfaces, and the energy position of the resonance reveals the bond length of the molecule on the surface.

Experiments in Europe and the USA on the photoionization characteristics of metal vapors are producing a clear picture of the photoexcitation process in transition and rare-earth metals. When the next-generation light sources become available, it will be possible to study multimetal clusters with and without ligands. These experiments will be seminal in identifying the degree of localization of the chemisorption bond on a surface and could be the key to understanding reactions on a finely dispersed catalyst.

Work is also being conducted on photoinduced fragmentation of molecules and transition-metal complexes; this work will have a direct impact on the understanding and the utilization of photon-stimulated desorption (PSD) from solids. In addition, this type of study suggests the use of tunable soft x-rays to stimulate selected chemical reactions that will selectively break large organic molecules.

A final example of the impact of gas-phase spectroscopy on condensed-matter science is the exciting photochemistry being investigated in Europe. This work uses a tunable synchrotron source to preferentially excite molecular ions to specific vibronic states. The ions are then allowed to interact with a second gas-phase species. This work, along with the work described in the previous paragraph, constitutes just the first sign of a new type of photochemistry.

2. The Impact of New Machines

In the future, the new insertion-device-based machines will have a great impact on gas-phase spectroscopy. The signal in most gas-phase-spectroscopy experiments is very low and will benefit spectacularly from the orders-of-magnitude increase in brightness that is offered by these insertion devices. In a gas-phase experiment, the sample density is approximately 10^{-10} times the sample density in an experiment involving a solid, and the required resolution is at least an order of magnitude smaller. For example, in many gas-phase experiments the output signal may be proportional to the machine brightness to the third power, so a 10^4 improvement in brightness would permit qualitatively new experiments. A simple argument will illustrate the dependence of the experiments on brightness.

For a given monochromator design, the output flux per unit energy resolution depends linearly upon the brightness of the source. If the ions or electrons being produced are to be energy analyzed, then the product of source area and accepted solid angle (brightness) is conserved in the analyzer, thus giving another measure that is linearly dependent on the brightness. Also, in many

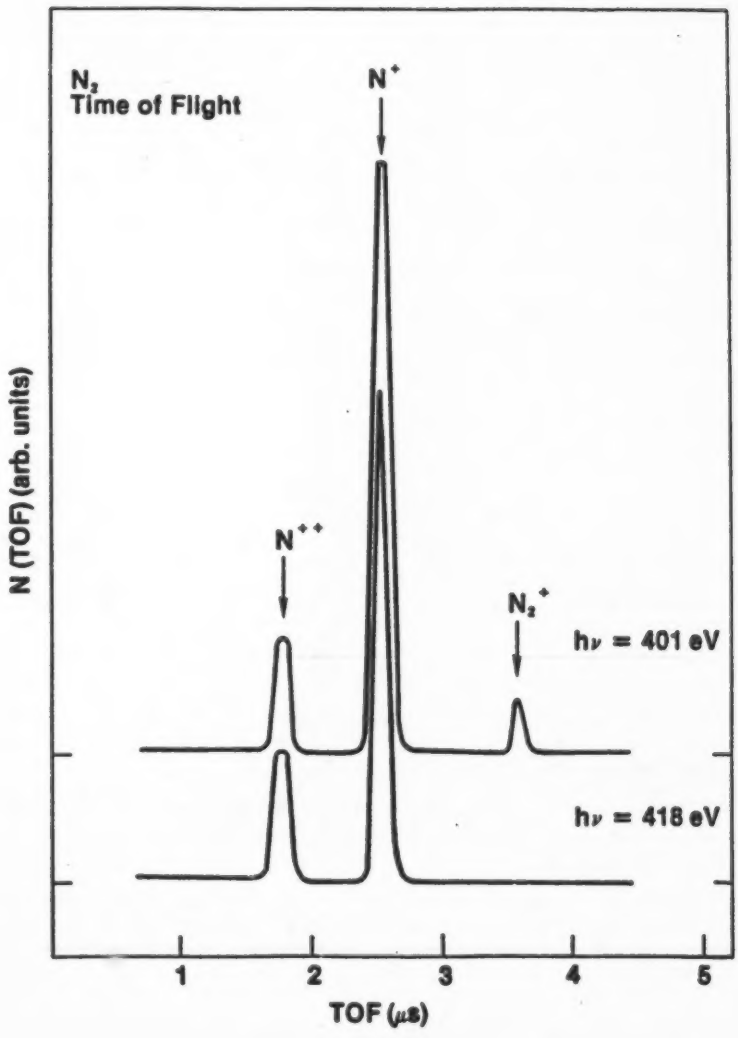

Figure 6. Ion-Fragmentation Patterns for N_2 Near the Nitrogen K Absorption Edge. The singly ionized molecule appears only at 401 eV, the molecular-nitrogen π resonance, where a direct-recombination process results in removal of only a single charge from the molecule. Other Auger decay processes lead to singly and doubly ionized atomic nitrogen.

future experiments, the amount of sample material may be very small, thus requiring small beams and a bright source imaged onto the sample region.

One prototype experiment will clearly illustrate the gains that are possible with the new sources. The core-level ion-fragmentation studies described above were carried out on a bending-magnet beamline. The counting rate for the ions produced was approximately 10 Hz in a peak, and the equivalent counting rate in the energy distribution of emitted electrons was approximately 1 Hz. These rates were accumulated with a photon resolution that was 10 to 50 times poorer than what was needed to fully separate features in the spectra. The experiment that one would like to do requires better resolution in both the incident light and energy analyzer and enough light intensity so that the electron-decay signal and the ion fragmentation can be run in coincidence while simultaneously measuring the kinetic energy of the ions. Such an experiment would require the brightness to be increased by a factor of approximately 10^4; it would also require a new monochromator that would produce an energy resolution of 1 part in 10^4 at a photon energy of hundreds of volts.

The new insertion devices will also create the following opportunities in gas-phase spectroscopy:

A. When a photon excites an atom or molecule, electrons, ions, and photons are emitted as a result of either the excitation process or the resultant decay. An in-depth picture of the dynamics of the process can be obtained by coincidence measurements. For example, coincidence between the energy-resolved electrons and the ion fragments can determine the decay channel. Ion/ion-coincidence measurements will relate the ion pairs in the fragmentation, and electron/electron-coincidence measurements can detect multiple Auger decay or relate structure in the Auger spectra to the initial excitation state.

B. It will become possible to study the electron energy levels and the lifetime of excited complexes by synchronizing a laser and the short time pulses from the storage ring.

C. The photoemitted electrons will be intense enough so that they may be run through a spin-polarization detector, which usually has an efficiency of 10^{-3} to 10^{-6}.

D. The proposal from LBL to couple a vertical and a horizontal undulator to "control" the polarization points the way to a technique that would allow the experimenter to easily investigate the "right" or "left" handedness of complexes.

E. It will be possible to use dilute supersonic beams or to investigate the interaction in crossed molecular beams.

In summary, these new and bright insertion-device sources will open up new frontiers in gas-phase spectroscopy for exploring in detail the geometric and dynamic properties of atoms and molecules in electronic states previously inaccessible.

Photon-Stimulated Desorption (PSD) -- PSD is a relatively new application of SR that has both promise as an analytical tool and the potential for provid-

ing some new insight into the energetics and dynamics of highly excited surface-bonding states. The analytical usefulness arises from the highly specific nature of the desorption process. Desorption occurs only from the surface layer and only from the surface-bonded complex that is electronically excited by the incident radiation. Thus, surface-and site-specific information can be derived for the desorbed species by analyzing the spectral dependence of the desorption (by means of NEXAFS and EXAFS), as discussed in the preceding sections on surface structure. Surface structure can also be directly analyzed through the study of ion-angular distributions. There are a number of important problems of fundamental and technological interest regarding which desorption can provide unique insight. Two examples of such problems are:

1. Catalysts and Catalyst Supports -- Catalysts in general have complex surface structures whose chemistry is dominated by minority sites. The site and adsorbate specificity of PSD allows the study of such complex surfaces in a direct way.

2. Hydrogen on Surfaces -- Hydrogen/surface chemistry is critical in a range of technologically important processes, including catalysis, corrosion, semiconductor processing, electrochemistry, ceramic processing, and many others. PSD is very sensitive to hydrogen and can not only define its bonding site but also determine the electronic and geometric structure of the site.

Because desorption cross sections are often extremely small and because systems of interest involve submonolayer coverages, PSD is one of the most "photon hungry" of techniques. In addition, many systems and processes of high importance--e.g., catalysis, corrosion, and ceramic powders--involve the study of small particles, requiring the use of a highly focused photon beam.

Desorption is now known to be induced by multiply excited states in which strong correlation effects lead to unique charge dynamics, which in turn can lead to both high-energy deposition on a site and electronic lifetimes of sufficient length for desorption to occur. Investigations of the physics of this effect will require examining systems with a range of desorption cross sections. One of the most potentially informative of experiments involves the measurement of ion/ion- and electron/ion-coincidence events. These studies require high flux, high spatial resolution, and timing capability. Coincidence experiments are not feasible with bending-magnet sources but could become feasible with insertion-device beamlines. An important adjunct to the desorption experiments is the study of photon-stimulated dissociation of large molecules. This research has had a direct impact on our thinking regarding radiation-induced damage and chemistry.

Imaging and Microstructure Fabrication

Soft X-ray Microscopy -- The term "x-ray microscopy" refers to a broad range of techniques that use soft x-rays to obtain morphological information about small objects. Biological and medical applications of microscopy are the most prominent applications, but others are emerging. The scientific value of these techniques derives from limitations in the present approaches to microscopy. Specifically, visible-light microscopy, electron microscopy, and hard x-ray crystallography all provide excellent imaging capability, but

they have various limitations. For example, consider a biological cell that is 1 to 3 μm wide and that contains interesting structures smaller than 1/4 μm. It cannot be crystallized. It cannot be viewed with visible light and can only be imaged in the electron microscope if it is dehydrated, sectioned, stained with (maybe even replaced by) heavy metal, and placed in a high vacuum. There are many life-science problems that require a more gentle probe to gather morphological information with less damage than would be done in the electron microscope and to allow the sample to remain in its natural, wet, living state in the atmosphere. Imaging with soft x-rays promises all this plus element discrimination using x-ray-absorption edges.

1. General Technical Requirements

It appears that a breakthrough in x-ray imaging will result from advances in the microfabrication methods developed by the semiconductor industry. Zone-plate lenses with a spatial resolution of 600 A are being fabricated, and values of 100 to 200 A are expected soon. This development opens the way to a range of soft x-ray imaging methods, provided that a suitable source is available. This source must have optimum output in the 20 to 50-A region (covering the O, C, and N K edges), and for imaging it must provide the highest possible coherent power. (This quantity is closely related to the spectral brilliance.) These requirements will be met by an undulator having a large number (e.g., 100 to 300) of periods and operating on a low-emittance storage ring of an energy between 1 and 2 GeV.

For example, the emittance of a spatially coherent, 30-A x-ray beam is $\epsilon_{30} = 2 \times 10^{-9}$ m.rad. 30-A photons emitted from a phase-space volume larger than $(\epsilon_{30})^2$ cannot be utilized. As a result 99.99% of the radiation from bending magnets is wasted in imaging experiments conducted on present storage rings; the next-generation storage rings and undulators are very important to this work.

2. Specific Experimental Methods

Table 2 indicates six of the more important methods of x-ray imaging and the improvements expected with the next generation of sources. Only one method (number 1) now gives useful biological results, but most of them will do so given the new sources. The most fully developed methods are numbers 2 and 3, which are already applied to biology. The three-dimensional methods will take longer to develop, but they are of considerably more importance.

3. Specific Examples of Research Problems That can be Approached through Soft X-ray Microscopy

The manner in which bone-matrix vesticles organize themselves and eventually determine the calcium structures that form bone is not well understood. It is expected that this process can be followed using calcium-specific x-ray imaging methods and understood with the help of calcium EXAFS studies, if necessary, on a pixel-by-pixel basis.

Nerve cells can be imaged by conventional means, but there is no easy way to distinguish a joint (a synapse) from a simple overlap. Thus, the "wiring diagram" cannot be understood. With the aid of element-specific x-ray imaging,

Table 2

Six Important Methods of X-ray Imaging

Technique	Promise	Disadvantages	$\frac{\Delta\lambda}{\lambda}$ needs (%)	Status with Present Sources	Next Steps Given New Sources
1. Contact	δ-50A*	2D thin specimens only, damage problems	2	successful biology in progress	3D refinements
2. Zone plate lens imaging	δ-100-200A (zone plate limited)	mainly 2D high damage	0.3	successful trials at δ-500A	achieve δ goal, faster exposures, mitigation of damage problem
3. Scanning through zone plate focus	δ-100-200A (zone plate limited), intrinsically low damage, integrated with computer	mainly 2D slow speed hence small field	0.3	successful trials at δ-3000A exposures of an hour or so	achieve δ goal, few second exposures, incorporate spectroscopy & microanalysis
4. Scanning reflection systems	δ-few x 10^2A some 3D capability, high speed	difficult to fabricate	none	trials at δ- 3μm with high contrast objects	achieve δ goal
5. Holographic microscopy	3D images δ-few x 10^2A	slow	0.1	trials at δ-1μm with high contrast objects	smaller δ shorter exposure with low contrast 3D objects
6. Soft x-ray diffraction	3D images δ-few x 10A	slow high damage	0.3	proof of principle stage	reconstructions from single exposure (axial res'n less good)

* δ = resolution

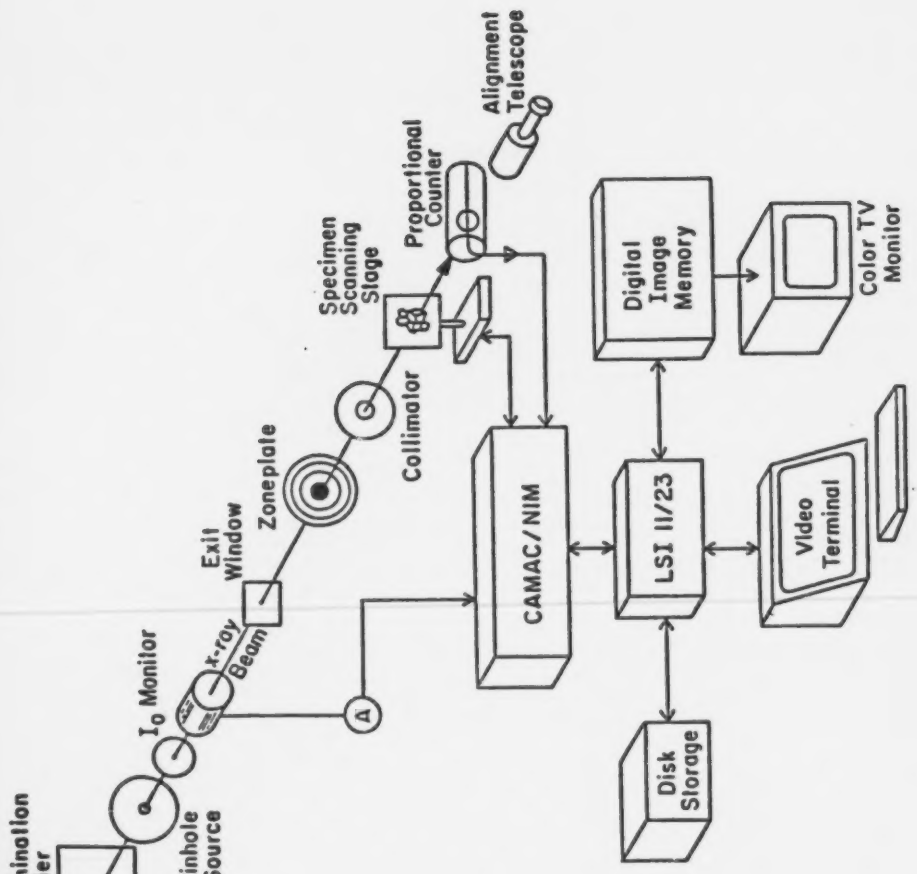

Figure 7. A Soft X-ray Microscope Utilizing a Zone-Plate Lens

it should be possible to highlight the synapses and thus follow the neuron-to-neuron connection sequence.

A similar three-dimensional structural problem is the elucidation of the arrangement of proteins, lipids, carbohydrates and water in ordinary biological cells. This basic problem cannot be solved by ordinary methods even in such well-known cells as blood platelets and bacteria. Bacteria have been chosen for a structural study that uses the C, O, and N K edges to give atomic specificity.

Microprobe Characterization -- Microprobe characterization of materials--an effort that includes both biological and medical applications--involves an investment of over $500 million nationally in electron microprobe equipment alone. However, x-rays have always been the radiation of choice for microprobe analysis because they provide the following advantages over electron excitation: a 10^3-better signal-to-noise ratio; cross sections that are higher by a factor of 10 to 10^2; reduction by a factor of 10^{-5} to 10^{-6} in the energy dissipated in the sample for the same detectable limit; improved accuracy in quantitative analysis; and the capability for measurements in the presence of air or H_2O (in vivo) with negligible charge collection. Historically, the low brightness of x-ray sources has prevented them from competing with electron sources, both because of the high brightness of the electron sources and because of the ease with which electrostatic and magnetic lenses collect and focus electrons.

With the advent of SR from insertion devices, the performance of an x-ray microprobe can exceed that of a microprobe based on electron sources. To cover the elements of the Periodic Table, an optimal x-ray microprobe requires a tunable undulator insertion device capable of delivering photon energies of from 2 to 33 keV. Obtaining energies of 33 keV from an undulator device requires circulating-electron energies of from 5 to 9 GeV, depending on the intensity of the higher-energy harmonics. Over the energy range of 10 to 33 keV, undulators in such a ring would deliver 10^3 to 10^5 times the intensity produced by current or soon-to-be-completed facilities.

The small angular divergence of the radiation from advanced insertion devices enables x-ray-diffraction techniques using crystals and multilayers to be used for collection and focusing. Thus, the demagnification achievable--just with present technology--would be about 100:1. As a result, spatial resolutions of 500 angstrom-diameters would be achieved in the analysis of bulk samples, as compared with the resolution attainable with an electron microprobe, which is limited by electron spreading in the sample to a level of 1 μm^2. Impurity levels on the order of parts per billion could be detected, compared to the limit of 100 parts per million with an electron microprobe. Diffraction studies of particles smaller than 60 A in diameter would be possible. Auger, photoelectron spectroscopy, and EXAFS analysis could be done in small selected areas of less than 1 μm-diameter. In summary, the x-ray microprobe would be a highly versatile tool, and many fields of research would benefit from its unparalleled performance.

X-ray Lithography -- The need for an alternative to optical lithography for manufacturing integrated circuits will probably occur in the 1990s, when it will become necessary to achieve a feature resolution of 0.5 μm. Electron-beam systems will be needed to make masks, but they will not be cost effective

for high-volume production in the direct-write mode. Synchrotron x-ray sources thus could become important tools for mass production of integrated circuits.

For microlithography, there are four basic requirements: resolution, registration, throughput, and defect density. Using optical lithography, it is now possible to make lines and spaces that are smaller than 1 μm and that are controllable to 0.1 μm. Optical techniques can be expected to attain a registration error of less than 0.25 μm between any two out of eight levels. In order to make x-ray lithography as economically desirable as optical lithography, processing must be done at a rate greater than 1 cm^2/s. Finally, the defect density must be less than one defect in 10 cm^2.

Several technological problems must be solved before x-ray lithography can be employed industrially to manufacture electronic devices. The technology for making an x-ray absorbing mask on a thin, x-ray-transparent, dimensionally stable support is probably the most important problem. Another problem involves simultaneously optimizing the source power and the resist sensitivity. Mechanisms for aligning the devices automatically during the exposure must be developed. Finally, a technology is needed for creating large (several square centimeters) high-transmission windows that can withstand the large pressure difference between the evacuated beamline and the lithography chamber.

1. Insertion Devices

The new high-brightness insertion-device synchrotron sources will allow the 4 to 14-A broadband range of the single bending-magnet source to be replaced with a bandwidth of a few percent that is centered at 15 A. Such a move favorably affects the mask-fabrication problem in that the gold-absorber thickness can be reduced from 0.6 to 0.2 μm, thus allowing 0.2-μm linewidths to be made with 1:1-aspect-ratio masks. Both wiggler and undulator insertion devices are sufficiently powerful and flexible to allow them to be used in an evolutionary way with conventional x-ray-tube technologies or in a revolutionary way at high-contrast, soft x-ray wavelengths (15 A). Wigglers would likely require a very thin (1/4 mil), high-power (10-W) window technology. On the other hand, undulator radiation is sufficiently compact (3 mm) so that differential pumping could be used instead of a window. The undulator also offers an additional degree of scientific sophistication that might ultimately be used to optimize the design of the beam while suppressing power load.

2. Throughput

Conventional x-ray-tube sources have required the development of very sensitive multilayer resist techniques. The throughput of these sources decreases quadratically with linewidth. Synchrotron sources do not suffer from the penumbra problem that underlies that loss and have consequently been pursued for the last several years.

To expose robust single-layer resists, an absorbed dose of 250 to 1000 J/cm^3 is needed in materials like PMMA. At 8 A this dose requirement translates to a flux of 0.25 to 1 J/cm^2 or $1x10^{15}$ to $4x10^{15}$ photons/cm^2. Because the x-ray optical-delivery system is only 13 to 17% efficient and because a writing speed of 2 cm^2/s is needed to compete with the optical throughput, a source of $1x10^{16}$ to $5x10^{16}$ photons/s is needed. This flux requires a 4 to 14-A band-

width for a single bending magnet at 400 mA and has led to a full-spectrum-synchrotron-source approach. The recent development of wiggler and undulator technologies offers the unique possibility of obtaining sufficient power from a very restricted bandwidth. It will be possible to tune the source so as to minimize other technological problems such as mask alignment.

3. Registration and Resolution: Mask Technology

With sources available to date, x-ray masks have required about 0.6 μm of gold absorber. Yet the major application of x-ray lithography will likely be in the 0.5 to 0.2-μm region, due to the success of optical lithography at larger dimensions. A gold absorber with a thickness of 0.6 μm will lead to very high aspect ratios in this region. By shifting to softer x-rays such as 15 A, the mask thickness can be reduced. How far the wavelength can be shifted depends on the window absorption, the mask-substrate absorption, the amount of mask heating, the amount of diffraction, and the resist.

The main limitation involved in going to 15 A is the absorption in the intermediate windows, in the mask support, and in the atmosphere on the way to the resist. Even a 1/4-mil beryllium window produces an almost 3-fold decrease in writing speed, and 1/2-mil windows are unacceptable. Mask heating actually favors the use of 15 A because for a fixed flux level of 100 mW/cm^2, the incident power on the mask at the exposure rate of the resist is three times higher at 15 A than at 8 A. Diffraction limits the mask to wafer spaces up to 17 μm for 0.2-μm resolution, but this is not a major problem.

Given a 1/4-mil 3-mm x 3-cm window, a high-throughput wiggler lithography system could be built using a neon-gas absorption dip as a filter. However, the energy of the ring may need to be reduced to help eliminate the hard x-ray radiation. For an undulator an opening of 3-mm diameter is sufficient. By using three 100:1-aspect-ratio tubes and differential pumping, a windowless system could be built. Undesired harmonics could be filtered out using neon and helium gas. More sophisticated filtering could be done by using magnesium or multilayer mirrors. Any of these undulator systems would compete with the present optical-system throughput of 2 cm^2/s.

Although either a wiggler or an undulator insertion device might be adequate for x-ray lithography, undulators would offer the prospect of differential pumping, the heat load on the x-ray optics would be much lower, and the power-load-to-output efficiency would likely be higher. Finally, from an engineering point of view, there is an interesting optimum-design problem involved in obtaining the desired beam properties from an undulator magnet.

Emerging Techniques

Inelastic X-ray Scattering -- Dynamic excitations whose energies are on the order of the ambient temperature (so-called thermal energies) play a special role in the physics of condensed-matter systems. Traditionally, excitations in this energy range, below say 100 meV, have been examined using both laser-based Raman and Brillouin techniques for long-wavelength excitations and neutron-scattering techniques, which can cover a larger range of excitation wavelengths. Fundamental limitations in conventional-x-ray-source flux, colli-

mation, and tunability have prevented x-ray techniques from developing the ability to resolve x-ray energy transfers below 1 eV.

The development of synchrotron sources, and particularly the improvements that will be made in the next generation of high-brilliance machines, will make it possible to establish inelastic x-ray-scattering techniques. Studies carried out so far indicate that inelastic scattering with 15-keV x-rays could be resolved at the 1 to 10-meV level, using back-reflection technqiues with spherically bent perfect silicon crystals. For better resolution, perhaps to below 1 μeV, nuclear-resonance scattering from crystals or multilayers made with the Fe^{57} isotope is under active consideration. The only fundamental limit to be discovered so far is the limit imposed by the available source flux per energy bandwidth. For a 1-meV bandwidth, undulator sources on a high-energy storage ring would produce 10^{10} to 10^{11} photons in a beam whose area is less than 1 mm^2. Such flux levels are considerably higher than those available using neutron sources, so one imagines that a wide range of applications will be possible.

1. Inelastic-Scattering Applications in Condensed-Matter Physics

X-ray techniques will be able to compete in many problem areas traditionally accessed by neutrons, such as the study of phonons between 1 and 100 meV in bulk crystals. However, for certain applications, inelastic x-ray techniques will be unique. These areas include (1) the study of collective electronic excitations to which the neutron does not couple, (2) the range of energy transfers above 200 meV, which is easily accessed with a 15-keV x-ray probe but difficult for the much lower-energy neutron, (3) excitations in disordered materials in which high neutron-energy transfer cannot be produced at small momentum transfer, and (4) the study of systems for which only small samples are available. In the last category, the study of the dynamics of two-dimensional systems should be revolutionized by inelastic x-ray scattering. It should be emphasized that there are, correspondingly, areas in which the neutron probes will remain unique. These include the regime of energy transfer below 1 meV and the study of magnetic excitations.

2. Inelastic X-ray Scattering Applications in Biology

Much of the importance of neutron scattering has derived from its applicability to the study of inelastic processes in solids. Furthermore, neutron scattering is an essential tool for studying hydrogen in biological systems. However, because of the low count rate and large sample size needed, inelastic neutron scattering has found somewhat limited application in biological materials. The development of inelastic x-ray-scattering techniques would have important application to the study of vibrational spectra in biological systems. For example, work on Raman scattering from proteins has suggested that there are anomalous features in the phonon spectrum as a result of a protein molecule being a pseudorandomly folded one-dimensional polymer. This is a kind of "fractal" structure. The understanding of this kind of behavior could help resolve the nature of intramolecular motions in proteins and polynucleotides.

Magnetic X-ray Scattering -- In considering the qualitatively new science that will develop with a high-brilliance source of hard x-rays, the possibility of magnetic x-ray scattering arises. There is a relativistic term in the x-ray-scattering cross section of atoms that is dependent on the magnetization

density. This magnetic scattering is weaker than the conventional Thomson cross section by the square of the ratio of the x-ray energy to the electron mass, which results in a factor of about 1000 for 15-keV x-rays. Further reduction in expected intensity results from (1) the number of magnetic electrons, which is usually small and always less than the total number of electrons, and (2) the form factor of the magnetic electrons, which falls off faster at high momentum transfer than the form factor representing the total charge density. As a result, the magnetic scattering from iron, for example, is weaker than the charge scattering by a factor of 4×10^{-6}. Although the magnetic effect is relatively weak, it should be easily observed with synchrotron sources, and magnetic scattering should mature into an important technique.

Preliminary experiments using conventional x-ray tubes and rotating anodes have succeeded in measuring magnetic Bragg peaks from antiferromagnetic and spin-density-wave materials at intensity levels consistent with the above estimates. On the basis of current experience with conventional charge scattering at synchrotron sources, it is clear that the next generation of high-energy storage rings will enable a variety of magnetic-scattering studies in bulk materials. These studies will have a number of advantages over neutron-scattering studies: (1) small samples (10^{-3} to 1 mm^3) will be quite adequate, (2) the higher resolution ($10^{-4} A^{-1}$) typical of SR will be routine, (3) materials with high neutron absorption (e.g., Cd or Gd) will be easily studied, (4) spin and orbital magnetization effects can be differentiated, and (5) anomalous magnetic-scattering techniques can be exploited. Perhaps more importantly, the intensity estimates are favorable for the study of two-dimensional magnetic structures and the surfaces of magnetic materials. The long-standing problem of surface-enhanced magnetism will be addressed, and it is possible that magnetic-reconstruction effects could be discovered.

Time-Resolved Techniques

1. Picosecond Timing in the Soft X-ray Ultraviolet (XUV)

Response-time measurements in the picosecond range open up a number of interesting possibilities. When a solid or liquid is excited (valence or core electronic excitation), a nonequilibrium-excited-state configuration results, and de-excitation leads to the production of phonons, photons, electrons, and sometimes displaced ions or atoms. Frequently, defects form and atomic rearrangement occurs around the excited atom. Over a period of time of about 10^{-16} second (corresponding to the absorption of radiation) to about 10^{-9} second (corresponding to the final decay processes in the vacuum ultraviolet [VUV]), a host of radiative and nonradiative de-excitations occur that include structural rearrangements. Very little is known about these various channels of decay, especially for core-level excitation.

The potential of a new timing technique, cross-correlation phase fluorometry--employing the short, repeated light pulses from an SR source was recently demonstrated in experiments to measure the luminescence lifetime of a number of organic and inorganic substances. In one case, a fluorescence lifetime of 196 ps was measured with an uncertainty of ± 6 ps. The technique is not constrained to lifetimes longer than the synchrotron-pulse duration. In fact, lifetimes as short as 0.05 ps might be measured with the new high-brightness sources, providing that the pulse structure is stable.

In addition to precise time-structure stability, high brightness is essential in timing experiments for at least two reasons. First, high intensity makes it possible to achieve good signal-to-noise ratios, especially with small samples. Second, highly collimated beams are important to reduce time spread or spatial dispersion in the picosecond regime.

2. Time-Resolved X-ray Scattering

High-resolution x-ray-scattering measurements performed at synchrotrons have yielded considerable insight concerning the equilibrium states of condensed matter. Time-resolved x-ray-scattering experiments will similarly enhance our understanding of nonequilibrium phenomena in liquids and solids. The problems that can profitably be studied using time-resolved techniques come from a variety of disciplines and have many practical implications. Examples are grain-boundary formation and growth in metals, melting, laser annealing, electrical switching, and phase separation in liquids and solid alloys. To date, very few time-resolved x-ray-scattering studies have been carried out. Nonetheless, these few studies have revealed dramatically new information, unavailable from other techniques, on laser annealing in silicon, phase separation in polymers, and switching in ferroelectrics.

The most important attributes that a synchrotron must have to make such studies feasible are high intensity and low emittance. The time structure of the photon flux is not particularly important because the photons are being used as probes of the systems under study. Detection technology borrowed from high-energy physicists will obviate the need to use a pulsed x-ray probe beam to time resolve the scattering data, even in very fast applications. A level of beam intensity that is higher than what is currently available will permit exploration of processes in systems--such as surfaces--with intrinsically small scattering amplitudes and of phenomena that cannot be reproduced at a sufficient rate to permit the use of present x-ray sources for the accumulation of statistically satisfactory data.

Time-Resolution Experiments in Biology

1. EXAFS on a Microsecond to Millisecond Scale

Current studies using energy-dispersive, time-resolved x-ray-absorption spectroscopy have achieved useful EXAFS spectra on a time scale on the order of fractions of a second. The increase in brightness on the order of a factor of 10^2 shows time resolution to be extended down into the submillisecond time scale. It should thus be possible to work on such a time scale in following conformational intermediates in photon-stimulated or chemically stimulated reactions initiated by a photolysis reaction. For example, it might be possible to study the unstable intermediates of the enzyme xanthine oxidase; in this enzyme, intramolecular electron transfer between the Mo site and the Fe/S center is thought to be on the order of or faster than 10 ms.

2. Study of Time-Dependent Phenomena in Biological Membranes

The use of time-synchronized detection in small-angle scattering has been demonstrated in Europe in studies on muscle function that were conducted on a millisecond-to-second time scale. The advent of higher-brightness sources should allow this technique to be extended into the submillisecond time range.

For example, the study of photocycling of bacteriorhodopsin at around 300 μs would be possible. A photocycle intermediate has been identified in this time scale by observing changes in the UV absorption spectrum after an initiating light flash. Accompanying structural changes could in principle be studied by performing a similar experiment using time-synchronized small-angle x-ray diffraction.

3. Single-Crystal Studies of Atomic Motions in Proteins

With current photon sources it is possible to use two-dimensional electronic detection techniques to collect intensity data for single crystals, on a time scale measured in the range of seconds to minutes. With higher-brightness sources, this time scale might be extended down into the ten-to-one hundred-millisecond time range. It is possible that certain thermally activated conformational changes in proteins, such as the flipover of a tryptophane side group, could be seen on this time scale by studying intensity fluctuations in various Bragg reflections. This kind of "noise spectroscopy" has been used to measure quantities like molecular weights in terms of fluctuations in a dielectric signal. An extension of this kind of fluctuation spectroscopy to x-ray diffraction would provide a new direction in biological-structure determination.

Applications

Metallurgy and Materials Science

Scientists and engineers in the fields of metallurgy and materials science comprise a community that is making increasing use of SR and that will become increasingly involved in developing new applications of this tool as new sources become available. This large community of new users has recognized the utility of synchrotron sources for diffraction, EXAFS, photoelectron-spectroscopy and x-ray-absorption measurements, topography, lithography, small-angle scattering, and flourescence analysis; but they have not been able to make extensive use of these techniques due to the unavailability of sources (particularly hard x-ray sources). Typical metallurgy and materials-science applications for which the synchrotron sources have unique advantages may be summarized in the following categories.

Diffraction and Scattering -- Structural analysis of small crystals or powders that are not available in the form of single crystals (e.g., zeolites and crystalline polymers) or small precipitated phases can be carried out. In fact, small crystals are often desirable for obtaining accurate electron-density distributions and for minimizing extinction and absorption. Alloy-structure determination for both crystalline and amorphous solids is an important area of future synchrotron research that will utilize the high resolution available in elastic-scattering experiments and the wide wavelength tunability that allows the use of anomalous scattering to selectively probe the structure associated with different elements. These SR capabilities allow studies of alloys comprised of near-neighbor elements in the periodic table.

Structural studies of clustering, precipitation, and spinodal decomposition will also be enhanced by the high brilliance of SR. It will be possible

to study the kinetics of phase changes, including fluctuation phenomena that characterize the early stages of many phase transitions. Studies of the time dependence of crystallization and of the liquid/solid phase change are important areas of investigation for many different types of materials.

The structure of two-dimensional phases such as those at grain boundaries is an ongoing subject of research in which the high brilliance, tunability, and high collimation of synchrotron sources will make important advances possible. For example, the study of metals and ceramics have shown that significant diffracted intensities can be obtained from the small volumes of materials at the grain boundaries.

Finally, the high brightness and tunability of the new sources will allow studies of diffuse scattering in systems that cannot now be adequately studied, such as ternary and quaternary alloys and polymer samples that are comprised of weak x-ray scatterers.

Topography -- Topography in both the white-beam and monochromatic modes will be extensively used to image lattice strains. In this application the methods are complementary to the more commonly used electron-microscopy methods. X-rays have a higher sensitivity to lattice strains and can be used to image larger areas of the specimen. Other novel applications will include time-resolved studies of plastic deformation and fracture using topographic imaging of line defects. Using high-brilliance sources, these studies will be able to determine lattice strains with a spatial resolution of a few micrometers. Experiments can be carried out in aggressive environments, and in situ studies of corrosion and oxidation will be possible.

Studies of the dynamics of phase transitions such as precipitation, solidification, and melting will be carried out by direct imaging; the same technique will be used to study the dynamics of domains in ferromagnets and ferroelectrics. Dynamic imaging of acoustic waves and of their interaction with lattice defects will also be possible, thus allowing the study of acoustic delay lines and filters.

Area-resolved EXAFS using wavelengths near an adsorption edge to form a white-beam topograph has been demonstrated and will allow correlations of the EXAFS data obtained from small-volume samples such as precipitates and grain boundaries. With extremely high-intensity sources, all these experiments could be done with a time resolution in the millisecond to microsecond range, thus making it possible to observe dynamical changes.

EXAFS and NEXAFS -- These techniques have a wide range of possible applications to metallurgical problems. Some of the more interesting possibilities involve investigation by fluorescent x-ray-absorption spectroscopy of the structures formed by relatively dilute (0.01% to 1.0%) solutes that influence the physical properties of steel and other alloys. Experiments of this type have studied internally oxidized Fe in Cu at a level of 75 ppm and have revealed that the structure differed from that of bulk oxides. Investigations of fine carbide, nitride, and carbonitride precipitates in high-strength low-alloy (HSLA) steels containing 0.05% to 0.2% Nb, V, or Ti have been carried out, and time-resolved techniques have been used to study the precipitation of Nb carbides in a steel.

SCIENCE AND TECHNOLOGY

Some of the many other metallurgical problems that are amenable to investigation using EXAFS/NEXAFS techniques are:

1. Investigation of the structure and chemistry of the complex precipitates that form in industrially important alloys. These studies will include the partitioning of solutes between the solid solutions and the several types of precipitates. Examples of such important precipitation systems are the complex alloy carbonitrides in HSLA steels.

2. The formation of complex oxides in stainless steels and other corrosion-resistant alloys is poorly understood. Through the use of high-intensity sources, EXAFS techniques may be applied to these problems. These measurements will be carried out in situ during oxidation or corrosion reactions.

3. Using high-intensity synchrotron sources, studies can be undertaken of the local atomic structure and chemistry of grain boundaries enriched by segregation of such elements as Sn, Sb, As, P, and S. These measurements can then be correlated with those obtained from studies of temper embrittlement in steels, of grain-boundary embrittlement in Ni-base alloys, and of hydrogen embrittlement.

Fluorescence Analysis -- New synchrotron sources offer exciting opportunities in the use of flourescence analysis to chemically analyze micrometer-sized areas; elemental sensitivities on the order of parts per billion would be possible for many important elements, including some of the important lighter alloying elements. Additionally, the x-ray optics developed for this technique will also allow the use of EXAFS and NEXAFS techniques on micrometer-sized regions.

Small-Angle Scattering (SAS) -- New synchrotron sources will enable significant advances in small-angle-scattering techniques. These techniques will be of great importance in studying the early stages of precipitation in many alloy systems. Particularly important applications will be made to polymer studies, and some of these have already been undertaken. Real-time acquisition of small-angle-scattering patterns at a data rate of 30 Hz has been accomplished and is being applied to the study of crazing in rubber-modified polymers and glassy polymers. Many other properties of polymeric systems, particularly their behavior under applied fields, will be better understood with the advent of these new techniques.

Phase-Transition Physics

One of the major achievements of modern condensed-matter physics is the general understanding of the phase-transition problem. In the context of this basic understanding, it is remarkable that so much remains to be discovered about the mechanisms and characteristics of various phase transitions. SR techniques have made important contributions to our understanding of these subjects, particularly in the heretofore virgin area of two-dimensional structural phase transitions. Generally, these SR studies have produced higher-quality data than have been obtained using conventional x-ray and neutron sources in studies of three-dimensional systems. The advantages here of SR are: 1) intensity levels high enough to get a reasonable scattering rate from

a single atomic layer and 2) high collimation of the beam, which permits the study of structural correlations involving lengths up to 1 μm. Some of the highlights of this research are described below.

The Absence of Long-Range Order in Two-Dimensional Crystals -- On quite general theoretical grounds, two-dimensional systems, unlike their three-dimensional counterparts, cannot develop rigorous long-range order. Although this concept has been understood theoretically for a few decades, no experimental verification of these effects was possible with conventional x-ray sources or with other probes. With the development of SR-based high-resolution scattering techniques, such studies have become possible. Detailed analysis of the diffraction line shapes obtained from freely suspended liquid-crystal bilayers and from incommensurate xenon monolayers adsorbed on graphite have documented these effects quantitatively.

Two-Dimensional Melting -- Experiments designed to follow the melting process in a two-dimensional layer, with temperature resolution of a few millikelvin, have been carried out on a number of systems, including variable-thickness liquid-crystal films and krypton and xenon monolayers (see Figure 8). Systems without a substrate and incommensurate systems show both first- and second-order melting behavior; the type of melting behavior that is shown in a particular case depends on the details of the system. A new phase in two dimensions, the so-called hexatic phase, has been seen in substrate-free systems, in multilayer systems, and in systems with an incommensurate substrate.

Commensurate/Incommensurate Transitions -- The influence of a substrate potential may lead to new phases in the phase diagram of a monolayer system. Specifically, the monolayer may be perfectly registered with the surface, or it may be incommensurate. When it is incommensurate, it may have its crystal axes either aligned or rotated with respect to the substrate axes. In cases in which the substrate is biaxial, the adsorbate system may be incommensurate in one spatial direction and commensurate in the other. All of these cases have recently been seen in various systems studied with SR, and transitions between them are under active study. One of the most unexpected discoveries in this endeavor was the observation that the commensurate/incommensurate transition proceeds through an intermediate, disordered, liquid-like phase. This phenomenon may have important consequences in the growth of ordered epitaxial structures.

Multilayer Phenomena and Wetting -- The structure of multilayer systems is as important as the structure of the surface and adsorbate layers. Important questions concern the transition from the nonwetting regime, in which only a few layers will adsorb below bulk coexistence, to the wetting regime, in which an infinite number will adsorb. Remarkable phase transitions occur in which, for example, a system consisting of one adsorbed layer and of bulk crystallites transforms to two adsorbed layers with correspondingly less bulk material. So far, this behavior has been studied for ethylene and oxygen adsorbed on graphite, and a great deal of work remains to be done in many other systems.

Biological Structure

Over the past decade, SR studies have played an ever-increasing and, in some cases, pivotal role in unraveling aspects of the molecular structure and

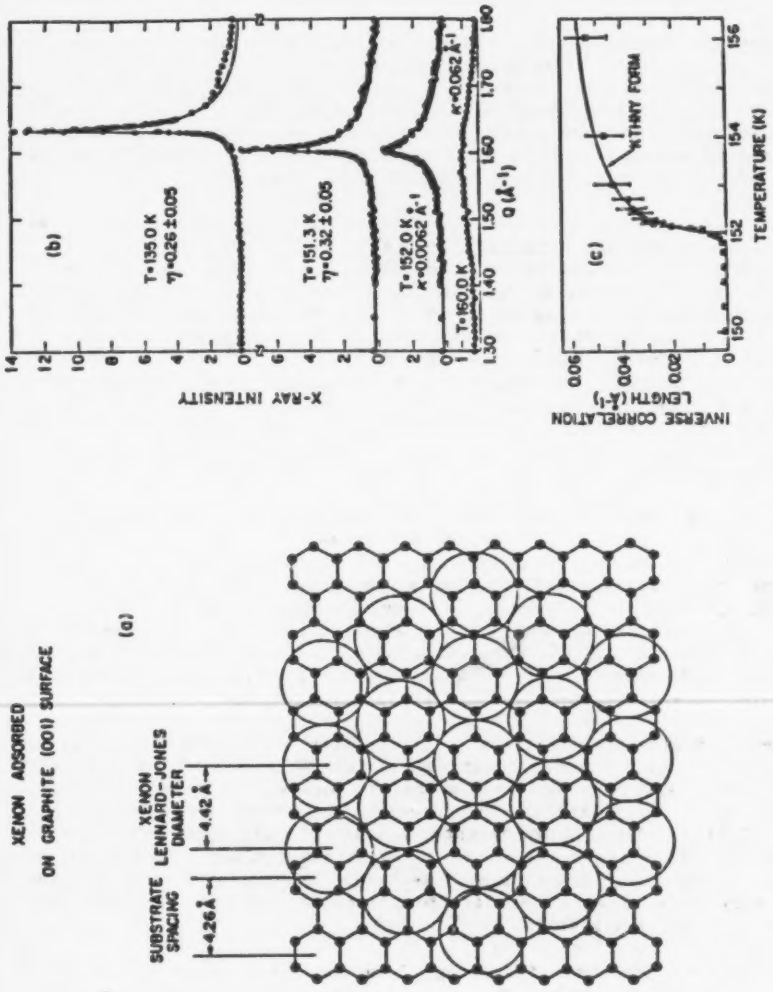

Figure 8. Melting of a Xenon Monolayer on Graphite. (a) An illustration of a monolayer of xenon adsorbed on the (001) surface of graphite. (b) Diffraction line shapes illustrating the absence of long-range order in the two-dimensional solid and demonstrating the continuous nature of the melting phase transition. (c) The measured temperature dependence of the inverse correlation length at the melting transition compared to a theoretical prediction.

function of biological systems. This has been true in studies of local structural environments of metalloproteins, using x-ray-absorption spectroscopy (NEXAFS and EXAFS); studies of macromolecular assembly and function, using small-angle x-ray scattering; and studies of three-dimensional protein structures, using crystallographic and anomalous-scattering methods.

X-ray-Absorption Spectroscopy -- The availability of SR revolutionized our ability to obtain useful information from x-ray-absorption spectra. EXAFS has proven its capability for determining the atomic arrangement around a specific atom in materials under physiological conditions. Distances can be determined to accuracies of within a few hundredths of an angstrom and coordination numbers and types can also be determined. Information about site symmetry and oxidation state is provided by edge analysis.

EXAFS and edge spectroscopy have demonstrated particular applicability to biological systems in which a metal ion is the site of catalytic action that results in the binding of a biologically active small molecule (such as dioxygen). For example, the enzyme nitrogenase is responsible for the conversion of atmospheric dinitrogen into ammonia, which can be assimilated by growing plants. Structural aspects of the molybdenum site in nitrogenase were elucidated for the first time by EXAFS (see Figure 3), thus stimulating activity toward synthesis of inorganic analogues. In chloroplasts, EXAFS has been used to help define the role of manganese in photosynthesis. Cytochrome oxidase is the terminal electron acceptor in the mammalian respiratory chain. Crucial questions about the nature of the iron and copper atoms in the enzyme have been resolved by EXAFS.

X-ray Crystallography -- X-ray-crystallographic studies provide virtually all of the information that we have about the three-dimensional structure of proteins and about how enzymes function on a molecular level. One of the most common problems in protein crystallography is obtaining crystals of sufficient size and stability to allow collection of three-dimensional diffraction data. SR studies in the USA and in Europe have shown significant enhancement in achievable resolution and significant reduction in the time required for such studies. It has also been found that some protein crystals undergo less radiation damage for a given dose if it is applied over a short time.

Recent developments in the ability to crystallize membrane proteins, using special detergents, enable the use of protein crystallography for the determination of the atomic structure of these proteins. However, a major difficulty is the production of sufficiently large crystals to obtain diffraction to a reasonable resolution. Use of high-brightness sources would allow measurements on crystals whose volume is on the order of 10^3 times smaller than the volume needed at the present time. A measurement technique capable of such resolution would find a very wide range of applications because many proteins can only be crystallized in very small sizes.

Another important technique involving the preparation of two-dimensional protein single crystals by adsorption to a lipid monolayer is opening up a new field of structure determination for biological molecules. Preliminary work has shown that it is possible to obtain well-defined diffraction peaks from adsorbed lipid monolayers on a crystalline substrate. The extension to crystals of macromolecules, such as proteins, has not yet begun. In the near future, it should be possible to repeatedly prepare 10x10 μm monolayers of

immunoglobulin crystals. The use of x-ray diffraction from such samples could allow the determination of structure at high resolution, for molecules that will not crystallize as three-dimensional structures.

Anomalous X-ray Diffraction Studies -- The use of anomalous scattering is gaining importance for biological-structure studies. Normally, the classical phase problem is solved in protein crystallography by means of multiple isomorphous replacement through soaking the crystals in solutions containing heavy-metal ions. By using multiple data sets, one from each heavy-atom derivative, the structure of the protein crystal can be determined.

The same information can be obtained by changing the wavelength of the x-rays around the absorption edge of an element already present in the sample. This technique is currently proving to be very useful in obtaining direct-phase information and thereby a solution of the crystal structure. The experiments are difficult owing to the small change in total effective electron density as the x-rays are tuned through an absorption edge: for lanthanide ions these changes, some of the largest known in any element, are in the range of about 20 electrons. The resulting change in diffraction intensity in a large molecule that may contain many thousands or tens of thousands of electrons is on the 0.1% to 1% level. In order to obtain a measure of such small changes with a sufficiently good signal-to-noise ratio, a very large number of counts needs to be taken.

A very high data rate is important because radiation damage is likely caused by migration of free radicals. Thus, it is advantageous to use a very-high-brightness source in addition to taking other precautions (such as rapid cycling of the sample through the beam) to minimize the effects of radiation damage. As the sensitivity of the technique is improved, new ways of labeling specific regions of molecules of interest may be developed, for instance by means of special lanthanide chelating agents that would bind in a controlled way to specific sites in a macromolecule. Anomalous diffraction could then be used to locate the marker group within the overall molecular structure.

Small-Angle Scattering -- Small-angle scattering is useful for studying the structure of biological molecules at intermediate resolution and for following changes in the structure as a function of time. One of the earliest uses of SR was to record time-dependent diffraction from a contracting muscle. The studies yielded information about the nature of cross-bridge action in the contracticle process. Studies of scattering from solution have helped define the way in which microtubules are assembled from subunits and the assembly of viral proteins into a capsid. The conformation of macromolecules in solution can also be studied as a function of biological effector.

Summary -- In summary, the availability of sources of increased brightness will open up new possibilities in the use of x-rays for biological-structure determination. The availability of an intense, highly collimated x-ray beam can be exploited in a number of ways. These all depend on selective use of the very high fluxes that can be made incident on a biological sample either in time, to give time-resolved diffraction information; in energy, to give increased ultrahigh resolution that can be used for inelastic studies; or in real space, to make it possible to get useful diffraction information from ultrasmall samples. The combination of high brightness and tunability available in an SR x-ray source will also make possible the use of anomalous x-ray diffraction on samples involving high dilution of an anomalous scatterer.

Medical Applications of SR

In the U.S. there are about 3-1/2-million people who suffer from symptomatic coronary-artery disease and about 1-1/3-million new heart attacks per year, half of which are fatal. Screening high-risk subsets of the population is currently ineffective because the tests are too insensitive, too risky, and too costly. The present reference standard for assessing the extent and the severity of coronary disease is the invasive coronary arteriogram, in which a catheter is inserted through an incision and an iodine-containing contrast agent is injected into the artery; radiographs, including cine images, are then recorded.

The properties of SR make it highly suitable as an x-ray source for use in a relatively safe and inexpensive approach based on iodine K-edge dichromography. A rapid scanning procedure is performed in which pairs of line images are recorded with monochromatic radiation above and below the K-edge of iodine (33.16 keV). The logarithmic subtraction of the two recordings results in an image whose sensitivity to iodine is about 39,000 times greater than it is to bone and about 170,000 times greater than it is to soft tissue. Preliminary recordings of the central circulation in anesthetized dogs provide good images of the major vascular structures and have demonstrated one of the coronary arteries, the left anterior descending artery, whose diameter in a dog is typically about 1 to 2 mm.

What will happen if future experiments on humans are successful? There is a high probability that there will be the need to develop compact, inexpensive, and widely available SR sources. These can also be used for other medical purposes. For instance, barium K-edge (37.44 keV) dichromography could result in a reduction in x-ray dose and in an increased information yield in studies of the gastrointestinal tract. A similar approach can be used for nonangiographic iodine-based procedures such as myelorgraphy, cholecystography, and urography. The extreme sensitivity of the K-edge dichromographic technique to iodine will allow a major reduction in contrast-agent dose in those patients who cannot tolerate conventional doses. Such patients include the elderly and patients with severe hypertension, poorly controlled diabetes, renal failure, and other disorders. Finally, tunable monochromatic imaging could increase contrast in any form of radiography, thus improving the information yield for a given radiation dose.

Catalysis

Heterogeneous catalysts represent one of the most complex class of materials that have been studied with x-ray-absorption spectroscopy. These materials can be classified broadly as either metallic or nonmetallic catalysts, and in both cases the catalytic components are generally distributed on high-surface-area insulating supports. Supported metallic heterogeneous catalysts have been more widely studied with x-ray-absorption spectroscopy, but nonmetallic systems (mostly oxides and sulfides) have received some attention. Both types of catalysts are important technological materials, and numerous industrial processes in the petroleum and chemical industries are dependent on them.

Supported Metal Catalysts -- The early EXAFS studies of supported metal catalysts were initiated in the period (mid 70s) when EXAFS was in its infancy.

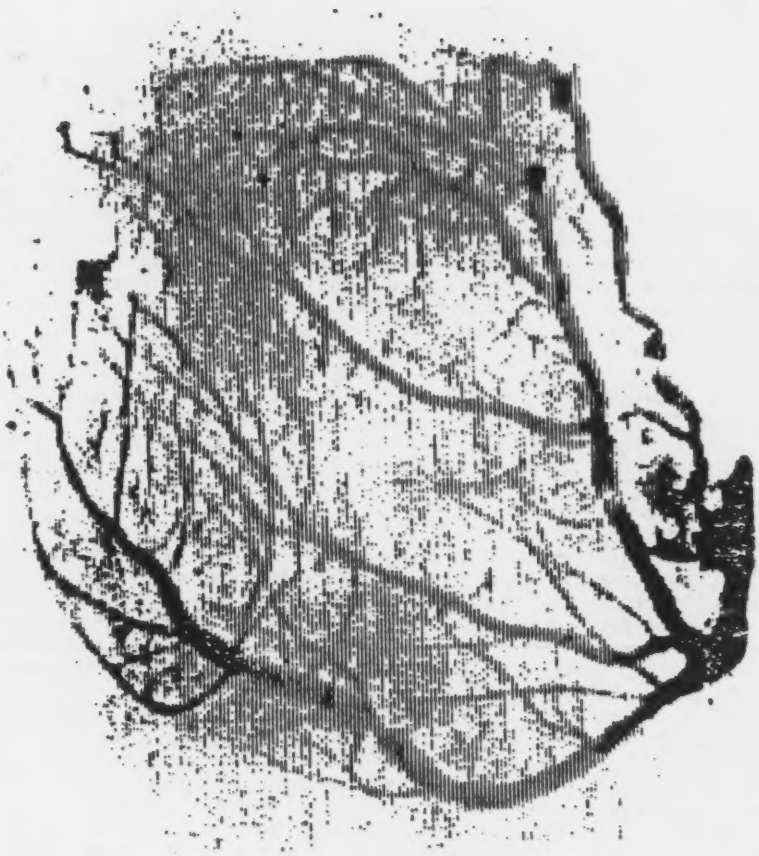

Figure 9. An Example of K-edge Dichromatography of the Arterial Structure of a Pig's Heart. Logarithmic subtraction of line images taken above and below the iodine K-edge yields greatly enhanced sensitivity to the arterial structure and discriminates against bone and soft tissue. Successful experiments have been carried out on anesthetized dogs.

The early work focused primarily on the structure of supported monometallic catalysts and for the first time provided catalytic chemists with detailed structural information on the small metal clusters that comprise these catalysts. Studies of the more complex supported bimetallic catalysts were undertaken following the early work on monometallic systems. Techniques were developed for analyzing these systems, and there is now a growing body of literature concerning the structure of these mixed-metal clusters. This work also contributed to the general development of EXAFS as an analytical technique by providing a body of structural information that could be assessed and compared to information from established catalytic-characterization techniques such as chemisorption, probe reactions, and electron microscopy.

Studies Under Reaction Conditions -- The use of SR for x-ray-absorption-spectroscopy studies of catalyst systems while reactions are actually occurring is an exciting development. The feasibility of such studies has already been demonstrated, and the resultant measurements will undoubtedly receive increased emphasis in the future. The possibility of relating the activity of a catalyst to structural and electronic properties of the catalytic system under reaction conditions is now at hand, and one can anticipate that such research will lead to a greater depth of understanding of catalytic phenomena.

With further experience in the use of SR in the study of catalysts and catalytic phenomena, one can anticipate that the volume of research will increase markedly. Although studies to date have been concerned primarily with basic-research programs on catalysts, an increased awareness of SR as a valuable tool in process- and catalyst-development programs in industry can be anticipated.

Zeolite Catalysts -- The activity and selectivity of zeolite catalytic materials are largely governed by their framework structures. Detailed structural information is then the key to understanding the properties of zeolitic materials. Unfortunately, most zeolites cannot be made in crystal sizes sufficiently large for conventional single-crystal x-ray structure analysis. Quantitative structural information is then only accessible through the use of powder-diffraction data. The averaging of the three-dimensional information limits the precision with which the structure can be defined.

High-brightness sources present the opportunity of accessing single-crystal diffraction data from very small particles--Micro-crystal Diffraction. In the first measurements obtained with this technique, data were taken from two cancrinite crystals with volumes of 13,000 μm^3 and 800 μm^3 respectively. These data demonstrate the feasibility of the technique and indicate that complete diffraction-data sets from micrometer-sized crystals should be routinely acessible. Owing to the severe limitations inherent in the use of powder data for structure solution, the application of synchrotron x-radiation in Micro-crystal Diffraction is expected to provide novel structural information on many catalytic materials, notably zeolites.

Earth Sciences

The application of SR to problems in the earth sciences is just beginning. It is clear that the many new studies that are possible with SR but not possible with conventional laboratory photon sources will have both substantial impact

in the earth sciences and important technological applications. Although the growth of this synchrotron effort has been severely limited by a lack of available beam time, a number of investigations have highlighted the areas in which exciting results can be obtained. The major applications to date mainly involve x-ray-absorption and -scattering studies.

Structure and Composition of Silicate Glasses -- The major purposes of this effort are to derive interatomic distances, coordination numbers, and concentrations for various elements in amorphous silicates. This work will improve understanding of structure/composition-dependent melt properties such as viscous flow, cation diffusion, and the solubility mechanism of volatiles (H_2O, CO_2) in silicate melts. Future work in this area will involve study of trace levels (<0.1%) of rare-earth, lanthanide, and actinide elements in silicate glasses and crystalline model compounds. In terms of geological importance, these studies have bearing on magma transport, eruptive mechanisms, crystal-melt element partitioning, element segregation in magma chambers, and melt growth of crystals. For certain glass compositions, these studies will also have bearing on nuclear-waste disposal.

Aqueous-Metal EXAFS -- This work has focused on the structure of metal complexes in concentrated aqueous solutions and on how this structure varies as a function of pH and ionic strength. Systems studied to date include electrolyte solutions involving Cr, Fe, Ni, Cu, and Zn cations and Cl and Br anions. Fluorescence EXAFS studies of ZnCl solutions at concentrations as low as 0.0001 M have been carried out. These concentrations approach those in natural hydrothermal solutions and in sea water, thus making it feasible to carry out speciation studies on the types of complexes that transport metal ions such as Fe, Ni, Cu, Ag, Au, and U in hydrothermal fluids emanating from cooling magma bodies and from midocean-ridge hydrothermal systems. These types of hydrothermal solutions are thought to be responsible for the transport and deposition of metallifferous ores that are so critical to our economy. Future work on geochemically important solutions should involve EXAFS studies at temperatures in the hydrothermal range (100° to 350°C). Our knowledge of the types of complexes present in heated solutions is currently limited to indirect information derived in part from solubility measurements. An important application of high-temperature (<100°C) EXAFS studies of aqueous complexes will be the study of radionuclide complexes such as those that could escape into heated groundwaters surrounding geologic waste-disposal sites.

High-Pressure/High-Temperature Phase Transitions and Equations of State -- One of the earliest applications of synchrotron x-ray work to geologic materials involved crystallographic studies of phases held at high pressure in diamond-anvil devices. With current technology, pressures as high as 1.7 Mb can be generated and held by such devices, permitting geochemists to model phases that might occur in the earth's lower mantle and outer core. Recently, simultaneous heating of pressurized samples has been accomplished to determine the equations of state of mantle materials. Because of the thickness of the diamond windows necessary for such experiments and because of the need for rapid measurements, these experiments are best done using synchrotron sources. Future work will involve scattering studies of oxides and silicates at pressure, in order to determine elastic constants. An exciting evolution of the current high-pressure/high-temperature phase-transition work involves time-dependent studies of the kinetics of phase transitions. One of the key theories developed recently for deep-focus earthquakes near plate boundaries involves mantle

phase transitions. However, questions concerning the kinetics of such transitions must be answered before these theories can be fully evaluated.

Powder-Diffraction Studies — Many geological materials occur in such small particle size that conventional structural characterization involving single-crystal techniques is not possible. Similar difficulty is faced with many synthetic materials, particularly those quenched from high pressures, that are used to model chemically more complex natural analogues or phases that may occur deep in the earth's interior but that are not naturally present in crustal rocks. Profile fitting of high-quality powder-diffraction data of such phases is essential for their structural characterization. Preliminary synchrotron studies have shown significant gains in resolution relative to the resolution obtainable using conventional sources; these gains will permit considerably more complicated structures to be studied. Future applications of powder-diffraction studies include phase-transition studies and the study of order/disorder relationships in minerals.

X-ray-Microprobe Analysis — There is a critical need to improve the detection limits for trace elements in geologic samples, while maintaining high spatial resolution for in situ analyses. The electron microprobe has revolutionized the study of materials, including those that occur naturally, and is capable of detecting elements with Z greater than 5 in amounts as low as 0.05 weight percent, with a spatial resolution of several square micrometers. Plans are underway to construct an x-ray analogue of the electron microprobe. Preliminary work has already shown that current technology is capable of producing a microprobe with minimum-detection levels of 1 to 10 ppm/s/m and a bulk-analysis system with a sensitivity of 30 to 100 ppb in a 1-minute irradiation. In situ measurement of trace elements will permit the study of trace-element partitioning among phases. Such data are essential for unraveling the origin of magmas and for studying their crystallization histories.

Structural Characterization of Metamict (Radiation Damage) Materials — A number of important geologic phases commonly occur in the metamict state due to the structural damage caused by the decay of radionuclides present in small amounts. An important example is the abundant mineral zircon, $ZrSiO_4$. These heretofore poorly characterized phases to some of the crystalline and amorphous materials proposed as hosts for waste radio-nuclides. The benefit of studying naturally metamict materials derives from the fact that the metamictization process in these materials has proceeded at natural rates, which are much slower than those realizable in the laboratory but which are similar to those that would occur in nuclear-waste repositories. Anomalous-scattering radial-distribution function (RDF) studies of these materials will also yield structural data that are complementary to those obtained using EXAFS.

Other Applications — Many other applications of SR to earth-science problems are possible within the next few years. Some important examples of such applications are: (1) x-ray-adsorption studies of melts, (2) characterization of mineral surfaces, including adsorption and desorption properties, using the surface techniques made possible by synchrotron sources, (3) the study of melting phenomena involving minerals, (4) the application of anomalous-scattering methods in the study of amorphous and metamict silicates, (5) the study of phase separation in geologic systems, using small-angle x-ray scattering, (6) single-crystal diffraction studies with superior signal-to-noise ratios and involving very small crystals, and (7) time resolution of transient effects such as those occuring during melting and during reactions of mineral surfaces with water and gases.

SCIENCE AND TECHNOLOGY

Plasma Physics

Plasma physics is an area with important defense, energy, and materials-technology implications. Studies of the optical properties of dense, hot (10^6 to 10^7 K) plasmas in the soft x-ray region have been very limited due to the high intrinsic brightness of the plasma. The ability to study hot and warm atoms and ions in both equilibrium and nonequilibrium conditions is crucial in the design of devices based on plasma interactions. Such devices are used in energy research, in the development of inertial- and magnetic-confinement fusion; in defense technology; in the study of such problems as arc formation in electrical switches and in flashover phenomena; and in the development of various plasma surface-processing techniques.

Undulators on a machine such as the Advanced Light Source (ALS) would produce x-rays that are unusually brilliant in the prime area of interest (100 to 1000 eV). In this energy range, the peak brilliance of the radiation from such an undulator would be greater than that of the radiation from a 1-keV Planckian, and this brilliance would make it possible to conduct studies on warm and hot atoms that heretofore could not even be contemplated. Above 10 keV even the radiation from wigglers on such a machine would be more brilliant than most laboratory-produced plasmas, and the radiation from undulators on a 6-GeV machine would far exceed the plasma in brilliance.

The new generation of SR sources would be very useful in the detailed study of dense plasmas. Diagnostics to measure Doppler broadening and even classical plasma interferometry would be possible, and measurements could be made at much higher frequencies than is currently possible. Plasmas with electron densities in the 10^{25} to 10^{27} e/cm^3 range would be transparent to x-rays at these frequencies (100 to 1000 eV), and thus undulator beams could be used as back-lighting sources. The beams could also be used to study bound/bound and bound/free absorption by highly ionized atomic species. Details of ionic populations could be measured, and x-ray-absorption coefficients of "warm" or "hot" atoms could be studied in detail.

Owing to the short pulse length and the high degree of linear polarization of these beams, the signal-to-background ratio could be substantially improved from the ratio attainable with conventional methods, which employ laser-produced plasmas to emit copious amounts of line radiation at restricted energies. Finally, the high brilliance of the new sources makes it possible to obtain the high spatial resolution required to perform such measurements as those described above.

Actinide Chemistry

The actinide or transuranium elements from Th to Lr constitute the least-understood chemical series due to their variety and high radioactivity. They are also, of course, of central importance in nuclear-energy development, nuclear-waste disposal, and nuclear-weapons technology. However, especially for the heavier elements of this series up to Es, the quantities available for study may be only in the milligram to microgram range. Effective source sizes are thus only 0.2 to 0.5 mm in diameter, with samples often being prepared in small capillaries. The extreme radioactivity of these materials also dictates that the sample be placed at least 1 meter from an external radiation source so that adequate safety shielding can be present.

Thus, although it is clearly of high interest to better study these elements and their compounds--for example, by photoelectron spectroscopy and other related techniques--achieving adequate intensities will require a special radiation source, particularly one with high brilliance in the VUV/XUV range. A source of sufficiently high brilliance could yield a beam of the requisite 0.2 to 0.5-mm diameter even at distances greater than or equal to 1 meter from the monochromator and could thus illuminate the specimen with full efficiency. It is estimated that such brilliances would have to be higher by a factor of from 10^2 to 10^4 than those of presently available SR sources, so that a highly optimized undulator-based source is suggested, such as those planned for the ALS. The optimum range of photon energy would be 20 to 600 eV so as to permit studying both valence (5f, 6d, 7s) and core (4f, 6p) levels.

Such a source would permit studying the gas-phase elements, the solid elements, and their compounds. Gas-phase atomic studies would provide an important reference point in determining the detailed electronic structure and in assessing the very strong relativistic effects involved. The rich multiplet structure expected in valence- or core-photoelectron emission from these elements would also require resolutions less than or equal to 0.1 to 0.5 eV to adequately resolve the features expected.

The types of measurements feasible would then include UV and soft x-ray photoemission, possibly in an angle-resolved mode. Two closely related photoemission measurements that could be performed are CFS and CIS spectroscopy. In the first of these techniques, a constant final state photoelectron energy is used with swept photon energy to map out initial-state density; in the second technique, a constant initial state energy is used with swept photon energy to map out final-state density. These materials would also be expected to exhibit "resonant photoemission," in which the photoelectron intensity from a given level exhibits abrupt changes as photon energy is swept through the binding energy of a lower-lying level; such measurements would provide very subtle information on the valence-state configuration and the valence/core interactions in those materials.

In compounds, it also would be of interest to do core-level EXAFS in order to determine bond distances. Particular features of the actinides that would be of interest include the atomic number at which the relatively weakly bound valence 5f electrons change so as to exhibit the behavior of the more strongly bound valence 4f electrons in the rare earths. Density-of-states measurements in solids, by means of photoemission, also would be of interest in locating the 5f levels, which lie very near the Fermi level. Finally, these materials might be expected to exhibit a different divalent state near their surfaces; this possibility could also be studied with these SR techniques.

In conclusion, studies of this very important and very poorly understood series of elements would be significantly enhanced by the availability of a next-generation VUV/XUV undulator source with high brilliance.

FACILITIES (USA)

Introduction

This section is divided into five major parts dealing with existing facilities, future facilities, cost projections for the development of future facilities, users, and important research and development (R&D) efforts that relate to synchrotron radiation (SR) facilities. The status of foreign SR facilities is described in Appendix B.

Existing Facilities

SR facilities in the USA that are in operation or are being commissioned are listed in Table 3 below.

Table 3

Existing SR Facilities in the USA

Institution	Name of Machine	Operating Energy
National Bureau of Standards	SURF II	0.28 GeV
University of Wisconsin, SRC	TANTALUS	0.25 GeV
University of Wisconsin, SRC	ALADDIN	0.75 to 1 GeV
Stanford University, SSRL	SPEAR	3 to 3.5 GeV
Cornell University, CHESS	CESR	5 to 5.5 GeV
Brookhaven National Laboratory, NSLS	VUV	0.75 GeV
Brookhaven National Laboratory, NSLS	XRAY	2 to 3 GeV

The following is a brief description of each of these facilities, giving the status of each as of the fall of 1983 and the individual plans for further development.

National Bureau of Standards--SURF II

SURF II is the USA's longest-operating synchrotron light facility, and it has some unique features. Unlike the other rings in the country, the electron orbit in SURF II is circular because it is contained between the poles of a single magnet. This circular electron orbit gives SURF II the capability of operating as an absolute-standard light source with which, given knowledge of the beam energy and position distribution in the orbits, the absolute intensity of the SR as a function of wavelength can more easily be calculated. The SURF II staff estimates that this calculation can now be done to an accuracy of 2% at a wavelength of 200 nm and to an accuracy of 3% at 4 nm. This accuracy is

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better than that required for the calibration of, for example, spectrographs used in astronomical research.

SURF II operates at 0.28 GeV with an initial current of 30 to 60 mA. Machine improvements over the last year in the rf, in the power-supply regulation, and in the vacuum are responsible for an increase to the present current level and an increase in beam lifetime. New monochromators emphasizing resolution and throughput are coming on line, as is a new high-resolution, angle-resolved electron spectrometer that is designed for use in gas-phase spectroscopy. This spectrometer involves a twice-standard-size spherical alalyzer with improved throughput at high resolution, and it employs three layers of magnetic shielding. There are currently eight experimental stations, with three more due on line next year.

University of Wisconsin--SRC (Synchrotron Radiation Center)

This laboratory has the 0.25-GeV ring TANTALUS, which has been in operation for some time, and ALADDIN, a 0.75 to 1-GeV ring that is now being commissioned.

In recent years TANTALUS has operated at a level of 95% of its scheduled time, which represents extreme machine reliability. The facility has been remarkably "user friendly" and serves as a model for other user facilities. Some of this success may be a matter of scale and thus may be difficult to maintain at the larger facilities characteristic of the future.

Like the vacuum ultraviolet (VUV) ring at the National Synchrotron Light Source (NSLS), the ALADDIN ring is designed as a second-generation SR source for research in the VUV and soft x-ray regions. It is designed with a low-emittance lattice that will give enhanced brightness to the bending-magnet source points, and it has four long straight sections (4 meters in length), of which at least two will be available for future insertion devices such as wigglers and undulators. This ring is now being commissioned, and many subsystems are being completed or developed. The 100-MeV Microtron injector is operating, and low-current beams have been injected into the storage ring and accelerated to 0.75 GeV. There are potentially 35 ports that can be developed from bending-magnet source points, and approximately 23 beamlines are now being developed.

Most of the eight monochromators now operating on TANTALUS will be shifted over to ALADDIN as part of the 23 devices that will be available in its early stages of operation. About half the monochromators belong to participating research teams (PRTs), and the other half are built and operated by the facility. A number of the new ALADDIN monochromators will operate in the difficult photon regime of several hundred to several thousand electron volts.

Stanford University--SSRL (Stanford Synchrotron Radiation Laboratory)

This is the largest of the presently operating U.S. synchrotron light facilities, and until the advent of CHESS, it was the sole source of harder x-rays. The SPEAR storage ring was built as an electron-positron colliding-beam machine for high-energy-physics research, and it continues to operate in this mode 50% of its operating time. (SPEAR currently operates a total of eight months out of the year.) When SPEAR is dedicated to high-energy-physics research, SSRL operates on a parasitic basis, and the beam energy ranges from

1.5 to 2.5 GeV, with beam currents of 5 to 25 mA. The remaining time the ring is operated in a dedicated mode for SSRL at beam energies of 3 to 3.5 GeV and with a typical current of 100 mA and a beam lifetime of between 10 and 20 hours.

SPEAR has many 2-meter-long straight sections that were originally used for beam-diagnostic and control equipment. Over the past several years, a program of modifications to the storage ring has made many of these straight sections available for insertion devices, and SSRL has pioneered the use of wigglers and undulators in such locations. There are now two 8-pole, 18-kG wigglers, a 60-pole variable-gap undulator, and a 54-pole variable-gap wiggler. The last two devices were constructed in collaboration with Lawrence Berkeley Laboratory (LBL).

Cornell University--CHESS

This facility operates parasitically on the high-energy electron-positron storage ring CESR, which typically runs at beam energy of 5 to 5.5 GeV. CHESS is the source of the hardest radiation available in the United States. There are six experimental stations, each accepting 14 mrad of light, on three beamlines. Until recently, typical currents were 15 to 20 mA, but recent modifications allow multibunch operation, and 75 mA in three bunches 870 ns apart is now anticipated. The bunches are very short (130 ps), and much of the research at Cornell has made use of this time structure in time-dependent studies.

A six-pole, 18-kG wiggler station is currently being implemented at CHESS. On it will be a carousel monochromator spanning 4 to 60 keV and a line for Bragg-Laue crystallography. In addition, there will be a large four-axis Huber instrument for accurate structure-factor measurements and for the electron-density mapping of crystals. Hard radiation will be employed for these studies so as to reduce the importance of extinction corrections.

Brookhaven National Laboratory--NSLS

The NSLS at Brookhaven National Laboratory is the first dedicated SR source in the U.S. with storage rings individually optimized for high brightness in the x-ray and ultraviolet (UV) regions. It is a national user facility, with user groups organized principally into PRTs; these PRTs have committed substantial resources and personnel to the construction and operation of beamlines on which they will utilize up to 75% of the operating time. (The remaining time is available to general users.) Representation in these PRTs includes 28 groups representing universities, industrial laboratories, and government laboratories.

The NSLS Phase I was a four-year construction project that began October 1, 1977. Groundbreaking occurred in September, 1978, and startup of the VUV ring took place late in 1981. Research at the VUV ring was underway by mid-1982. The XRAY storage ring is now in the commissioning stage and is expected to provide photons to users within the next few months.

The VUV storage ring is a four-superperiod machine of 51-meter circumference. Its principal design parameters are an energy of 700 MeV and a

circulating beam current of 1 A. It now operates at 750 MeV and has achieved a peak beam-current value of 300 mA and a source-brightness value of approximately 4×10^{13} photons/s·mm^2·0.1% bandwidth. Each superperiod or ring quadrant consists of a 90-degree bend section with optical characteristics that are favorable for achieving minimum beam-emittance values and that permit greater freedom for installing undulators or wigglers in the straight sections without adversely affecting the storage-ring beam parameters.

The four connecting long straight sections (each 3.2 meters in length) are used as follows: One is used for beam injection, one is used for an rf station, and two are used for insertion devices. One of these last two sections is now used for a 38-pole permanent-magnet undulator, which has been installed and operated and which is now being instrumented for usage in the 100 to 1000-A range. It provides for a potential brightness increase, compared with a VUV bending-magnet arc source, of approximately a factor of 100.

The photon beams are transported from each VUV-ring bending magnet, with a radiation fan of 75 to 90 mrad. The fluence is approximately 10^{14} photons/s·mrad·1%($\delta\lambda/\lambda$) at the critical wavelength of about 25 A (750 MeV). Under design conditions, the maximum source brightness at approximately 1-keV photon energy is 3×10^{14} photons/s·mm^2·1%($\delta\lambda/\lambda$) for the VUV-ring arc source. There are presently 13 ports being used or developed, and they split into two or three beamlines. By the end of 1983, there should be 18 beamlines in use or being commissioned, with 6 more under construction.

The thresholds for the various modes of instability for the NSLS rings have been calculated, and corrections have been designed. The dominant instability mode now encountered in the VUV ring is the longitudinal coupled-bunch instability mode, caused by the beam in conjunction with the rf-cavity parasitic-mode impedances. Therefore, a one-or-three-bunch mode of VUV-ring operation has been established, which, for one-bunch operation, results in a (present) maximum current of 300 mA but also in greatly improved beam stability and source brightness. Future improvements in the source emittances should result from a resurvey and realignment of storage-ring magnets during the next long shutdown, and the overall current values should improve after a tune-splitting cavity is installed this winter.

The XRAY ring, which is 170 meters in circumference, is similar in optical design to the VUV ring. However, it is comprised of eight achromatic bend sections, thereby providing a greater number of straight sections for insertion devices. The operating energy will be 2.5 to 3.0 GeV, and studies are in progress regarding the use of a new booster synchrotron to raise the injection energy to the operating energy. The XRAY ring has already operated at up to 2 GeV in beam energy with modest beam lifetime and beam current. A commissioning program is in progress to enhance the beam intensity and to align the external photon lines with the photon fans emerging from the XRAY ring. Seventeen front ends are operational, and 25 "hutches" are assembled and are being outfitted with experimental equipment.

The maximum radiation fan in an x-ray port is 50 mrad, which is typically subdivided into two or three beam lines. The maximum integrated photon flux for the XRAY-ring design parameters of 2.5 GeV and 0.5 A is 3×10^{15} photons/s·1%($\delta\lambda/\lambda$)·0.5A at the critical wavelength, for an arc source, of 2.5 angstroms. A superconducting wiggler at 50 kG would extend the spectrum into the hard x-ray

region with a flux (at a photon energy of 100 keV) of 10^{14} photons/s·mrad·1% ($\delta\lambda/\lambda$) at 500 mA.

General Summary

There continues to be rapid growth in the number of facilities coming on line for research in both the VUV and x-ray regimes. Although the needs of the community are for more sources at all energies, there will be larger increases in the number of beamlines for VUV and soft x-ray research.

The new facilities, including insertion devices on existing machines, will make available much brighter sources than those of the past. This progress, combined with the technological development of beamline design and instrumentation, is opening up new fields of research and enhancing the capability for research in the many areas of science that presently use SR.

Some of these facilities are taking longer to become operational than the SR community had expected. The problems have not involved technical considerations but rather a lack of resources, both manpower and money. Although the rings being built are physically smaller than those built for high-energy physics, they are equally complex and technologically challenging. To build and commission them on an expeditious schedule requires not only adequate funding but also a larger well-managed team of accelerator physicists and engineers than has been available on some recent projects.

FACILITIES (USA)

Future Facilities

The following table lists the new U.S. SR facilities that are being constructed, have been proposed, or are being designed or considered.

Table 4

Future SR Facilities in the USA

Funded and under construction	
Brookhaven National Laboratory	NSLS Phase II
Stanford University	1-GeV FEL storage ring
Stanford University, SSRL	SSRL Enhanced Photon Flux Facility (SEPFF)
Active Proposals	
Lawrence Berkeley Laboratory	1.3-GeV Advanced Light Source (ALS
Under Design or Consideration	
Brookhaven National Laboratory	NSLS Phase III 6-GeV Facility
Stanford University, SSRL	6-GeV-Ring Facility
Cornell University, CHESS	High-Energy Ring

These projects are described briefly in the following, in the order in which they appear in the table.

Brookhaven National Laboratory--NSLS Phase II

The NSLS Phase II Construction Project is made up of two basic components: 1) beamline construction, involving the development and installation of at least six additional beamlines and associated insertions; and 2) conventional construction, involving expansion of the existing NSLS building. Briefly, the objectives of the project are to:

- design and build six state-of-the-art beamlines with emphasis on wiggler and undulator insertions
- provide laboratory and experimental support areas to accommodate up to 80 beamlines
- provide integrated work and office space for 128 NSLS personnel.

Proposed Insertion Devices and Experimental Beamlines -- Six beamlines and three insertions* will be designed and built as part of the Phase II Construction project (Table 5). The locations of these beamlines and insertions on the XRAY and VUV storage rings are noted in the table. The first three beamlines in the table were proposed to the scientific community as pertinent to the community's current needs and have been endorsed by the Users' Executive Committee. The NSLS Department Chairman has approved them for early construction. The remaining three beamlines will be reviewed by user groups and then approved for construction by the NSLS Department Chairman no later than July 1984.

Table 5

Experimental Beamlines and Insertions,
NSLS Phase II Construction Project

Beamline	Insertion Device
Superconducting wiggler	Superconducting wiggler
High-Q-resolution x-ray	Hybrid wiggler
X-ray microscopy and holography	Soft x-ray undulator
Infrared	None
TOK soft x-ray	Multipole wiggler
High-Energy-Resolution inelastic x-ray scattering	Hybrid wiggler

Stanford University--1-GeV FEL Storage Ring

This 1-GeV storage ring has been designed specifically for the study of free-electron lasers (FELs) and is not primarily planned to be used as an SR source. However, the present design includes locations for up to four insertion devices, and SR research in the soft x-ray region and basic accelerator-physics research are planned as secondary uses.

Stanford University, SSRL--SSRL Enhanced-Photon Flux Facility (SEPFF)

In addition to a plan to increase the number of beamlines from both bending magnets and insertion devices over the next several years, there are several other improvement programs underway as part of SEPFF. They include: (1) machine lattice modifications that could reduce the dedicated-mode beam emittance by a factor of three, thereby increasing the brightness from all sources; (2) changes in the beam-control systems, to improve the stability and control of the electron orbits; (3) construction of a new alternate injector using only a small

*The superconducting wiggler has already been constructed. The transverse optical klystron (TOK) insertion magnet will be built with non-NSLS funds.

fraction of the Stanford Linear Accelerator Center (SLAC) linear accelerator. This new injector will allow the running of SPEAR in the dedicated mode during shutdowns in the SLAC high-energy-physics program, thus providing a 50% gain in running time; (4) construction of additional office space and assembly areas; and (5) the addition of an undulator to the PEP electron/position storage ring.

The PEP storage ring is operated by SLAC for the study of elementary-particle physics. In its present configuration, it can be usefully run at an energy of from 8 GeV to 18 GeV, although the majority of the program has focused upon activities at 14 GeV. During the normal running of the machine, the electron and positron beams emit SR from within the bending magnets with photon energies in excess of 100 keV.

More important to the SR community, however, is the fact that there are six 4-meter-long "symmetry straight" sections, many of which can accommodate wiggler or undulator magnets. In fact, three of the straight sections have 2-meter wiggler magnets already installed for the purpose of increasing the machine luminosity at low machine energies. The plan is to install in the first of these sections (symmetry straight #5) a 2-meter undulator in tandem with the existing wiggler magnet. Should the machine be run in a low-energy configuration, the diffuse wiggler radiation will be superimposed, to some extent, upon the undulator radiation, but this should create no unwanted background.

The design parameters were chosen to produce 12-keV radiation at the nominal PEP operating energy, 14 GeV, but the undulator will also produce extraordinary brightnesses at both lower and higher machine energies, as illustrated in Table 6.

Table 6

PEP-Beam-Facility Design Parameters

Electron Energy (GeV)	Electron Current[a] (mA)	Electron Emittance[b] $(m \cdot rad)^2$	Fundamental Energy (keV)	Photon Flux[a] $(sec^{-1} \cdot [100\%BW]^{-1})$	Spectral Brilliance[c] $(sec^{-1}[100\%BW]^{-1} \cdot mm^{-2} \cdot mrad^{-2})$
10.0	20.0	0.273×10^{-7}	6.080	2.87×10^{16}	2.66×10^{18}
12.0	24.0	0.567×10^{-7}	8.755	3.45×10^{16}	1.54×10^{18}
14.0	28.0	1.050×10^{-7}	11.917	4.03×10^{16}	1.09×10^{18}
16.0	32.0	1.791×10^{-7}	15.565	4.60×10^{16}	0.65×10^{18}
18.0	36.0	2.869×10^{-7}	19.699	5.17×10^{16}	0.46×10^{18}

[a]For dedicated operation, increase by a factor of 3.3
[b]For dedicated operation, increase by a factor of 9
[c]For dedicated operation, increase by a factor of 3.3 x 9 = 30

The first component of the beamline is the undulator, whose specifications are given in Table 7. Its design will be the hybrid samarium, cobalt, and steel design originally developed by Halbach. The vacuum chamber will be of the fixed-gap design, with an interior aperture of 36 mm and an overall thickness of 45 mm. The undulator will have a variable gap ranging from a minimum of 45 mm to a maximum of 100 mm.

Table 7

Specifications for the PEP-Beam-Facility Undulator

Magnet gap	45 mm minimum (variable)
Electron aperture	36 mm (fixed)
Magnet period	72.58 mm
Peak magnet field	2.239 kG (maximum)
K parameter	1.518 (maximum)
Material	SmCo, steel

The beamline will immediately be ready for high-resolution scattering and diffraction experiments. It should be noted, however, that the unique properties of the PEP-undulator radiation will make it possible to explore, as research-and-development projects, alternative configurations that will optimize the beamline for, e.g., Mossbauer diffraction and high-energy-resolution x-ray scattering.

The schedule calls for the approximately 3000-ft^2 building (and the interconnecting beamline tunnel) to be built during the PEP summer shutdown in 1984; the beamline components will be installed in the summer of 1985.

Lawrence Berkeley Laboratory--1.3-GeV Advanced Light Source (ALS)

The design of the ALS has been optimized to achieve two major goals: to provide intense photon beams in the energy range of from 0.1 to 5000 eV and to provide very short pulses (20-ps duration) of synchrotron light for the many experiments that are performed in this energy range and that involve timing requirements. At a reduced flux, pulses of as short as 5 ps could be available under certain operating conditions. The use of a superconducting wiggler could provide useful fluxes of photons at higher energies, e.g., 40 keV.

To meet these design goals, the electron beam has a very small design emittance (7×10^{-9} m·rad), and the ring has twelve 6-meter-long straight sections for wigglers and undulators. The low emittance, which is an order of magnitude smaller than that of existing machines, makes it possible to optimize performance from the undulators in the soft x-ray region and to minimize power loading on optical components in the beamlines.

All told, 30 or more photon beamlines (user ports) would emanate from the ALS's complement of 12 insertion devices, and a comparable number of beamlines could originate in bending magnets. According to the proposal, half of the insertion devices and beamlines would be built as part of the main construction project, with the remainder being developed by affiliates or PRTs. Table 8 summarizes the parameters of the ALS design, and Table 9 gives the project cost estimates. The insertion devices included in the project costs are listed in Table 10.

LBL has had a pioneering role in insertion-device development and has done a great deal of work in beamline design relating to the ALS and to the problems

associated with very high brilliance and high power density. The laboratory has recently formed the Berkeley Center for X-Ray Optics, where these problems, along with the development of x-ray instrumentation, will be intensively pursued. LBL has a large, highly qualified team of machine physcists, engineers, and technicians; they have had an important role in synchrotron development in this country.

Table 8

ALS Design Parameters

INJECTION	50-MeV Linac 1.3-GeV Booster
STORAGE RING	Design current (400 mA) Beam lifetime (> 8 h) Emittance (7×10^{-9} π·m·rad) Filling time (approximately 3 min) 12 (6-meter) straight sections (> 30 branch lines possible) 24 bending magnets (>30 branch lines potential)
GENERAL-USER PHOTON BEAMLINES (Construction Project)	4 undulators 2 wigglers 14 branch lines

Table 9

ALS Construction Cost Estimates[a]
(In FY83 Millions of Dollars[b])

Accelerator systems		**26.5**
Storage ring	11.7	
Injector	7.2	
Control system	2.6	
Contingency	5.0	
Beamline systems		**26.4**
Insertion devices	7.2	
Photon beamlines	14.2	
Contingency	5.0	
Conventional facilities		**10.4**
Removals and site preparations	2.2	
Building addition	2.7	
Shielding	1.8	
Utilities	2.4	
Contingency	1.3	
TOTAL		**63.3**

[a]Including project management, engineering, and design costs
[b]Does not include escalation

Table 10
Summary of Currently Planned ALS
Insertion Devices (1.3 GeV)

Name	Insertion-Device Type	Peak Field (tesla)	Period (cm)	Number of Periods	Length (meters)	Energy (eV)
U_A	Permanent-magnet undulator	0.39	16.7	30	5	5 to 700
U_B	Hybrid undulator	0.74	6.25	80	5	25 to 1500
U_C	Hybrid undulator	0.54	5.0	100	5	75 to 3000
U_D	Hybrid undulator	0.57	3.5	142	5	200 to 5000 (>10,000 at 1.9 GeV)
W_E	Hybrid wiggler	1.60	10.0	25	2.5	0.1 to 10,000
W_F	Superconducting wiggler	5.0	14.0	14	2	1 to 10,000 (>40,000 at 1.9 GeV)

Brookhaven National Laboratory--NSLS Phase III 6-GeV Facility

NSLS Phase III includes the construction of a 6-GeV, 5-mA booster synchrotron and a 6-GeV high-brightness "undulator/wiggler" electron storage ring. This construction program is planned in two stages. The first stage involves upgrades to the existing facilities and construction of the booster synchrotron, referred to as Booster II in the following discussion. Booster II will be used as a full-energy injector into the upgraded existing XRAY storage ring. Construction of the high-energy "undulator/wiggler" storage ring will follow as the second stage of the program.

Plans for the design, siting, and commissioning of Booster II have been made in such a manner as to make use of the existing linear-accelerator and booster as the injection system. Booster II will be located where construction and commissioning will not interfere with ongoing operations.

The existing XRAY ring was designed for a maximum energy of 2.5 GeV; however, easy upgradeability to 3 GeV was allowed for. The dominant component involved in increasing the energy to 3 GeV is the addition of rf acceleration stations. Additional rf cavities are presently in the construction stage. With the presently installed rf power amplifiers and a complement of four rf cavities, a beam energy of 3 GeV, with a 300-mA circulating beam, can be achieved.

There is a growing consensus that, in the coming years, a high-energy ring, operating at an energy on the order of 6 GeV, will become increasingly attractive for a variety of experiments. Thus, the Booster II synchrotron will not only be capable of injecting into the energy-upgraded XRAY ring, at an energy of 3 GeV, but it will also be designed to accelerate electrons to 6 GeV for full-energy injection into the high-energy "undulator/wiggler" storage ring to be constructed in the second stage of the program.

The basic parameters of Booster II are as follows:

Energy	6	GeV
Circumference	340.3	meters
Magnetic radius	26.7	meters
Beam current	5	mA
Radio frequency	370.2	MHz

Because the initial operating energy will be only 3 GeV, construction of a good fraction of the rf hardware could be postponed. It is desired, however, to avoid subsequent interruptions of the XRAY program; therefore, the full rf-cavity complement will be installed during the first stage of the construction program.

The siting and construction of Booster II and its associated tunnels and service buildings would have to take into account the subsequent construction of the 6-GeV undulator/wiggler (U/W) ring, which would have to be carried out with no interruption of the XRAY-ring experimental program. Reinjection of the 3-GeV Booster II beam into the XRAY ring has been examined in a preliminary manner. In crossing the XRAY experimental area, the charged-particle beam transport would pass under a number of photon lines in a manner analogous to what is presently done with the transfer line from Booster I to the VUV storage ring. Table 11 provides cost estimates for the various components involved in the construction of Booster II.

In order to improve the present charge-transfer rates into the VUV and the XRAY rings (and, from a longer-range point of view, into the U/W ring), an improvement program to increase the prebunch intensity in Booster I is being carried out. This program involves not only incorporation of a new state-of-the-art gridded electron gun but also the rebunching, at 800 MeV, of five bunches into one bunch, by means of a new 10.6-MHz rf unit. As a result, significantly shortened charging times will be achievable in the two existing storage rings, and, after completion of the U/W ring, charging of the three rings from zero circulating beam to design current values would be done in significantly less than 30 minutes.

A preliminary study of the high-electron-energy U/W storage ring has been carried out with the objective of potentially providing for ultimate-brightness radiation sources in the hard part of the x-ray spectrum. The design parameters were guided toward the use of a 0.86-A first-order spectral peak from a state-of-the-art permanent-magnet undulator source. These considerations led to a maximum electron energy of 6 GeV. While still keeping economic factors in sight, the design of this storage ring was optimized for minimum source emittance, thus resulting in the principle parameters shown in Table 12.

With its superperiodicity of 16, this ring would permit the ultimate use of $(28-N_W)$ undulators, N_W wiggler sources, $(32-N_{WS})$ dipole sources, and N_{WS} short wiggler sources. Table 13 gives more detail on these potential sources and compares them with those of the "P-ESRF," the European Synchrotron Radiation Facility, which is proposed for construction at a cost of approximately $150 million.

Table 11

Cost Estimates for the Construction of Booster II: NSLS Phase III
(In FY85 Millions of Dollars)

A.	Engineering, Design, and Inspection		5.50
B.	Booster II		
	1. Principal Systems		14.76
	2. Associated Equipment		1.48
C.	Conventional Construction		4.87
		Subtotal	26.61
D.	Contingency at 20%		5.32
		TOTAL	31.93

Table 12

NSLS High-Energy U/W Ring
Preliminary Parameters

Energy (GeV)	6
Periodicity	16
Circumference (meters)	753.58
Bending Radius (meters)	33.40
ν_H, ν_V	-25, -9
Momentum Compaction, α_P	4.5×10^{-4}
ε_H(m·rad)	0.7×10^{-8}
ε_V(m·rad)	7×10^{-10}
Dipole Field, B(kG)	7.5
Sextupole strength, B'' (kG/m^2)	-120
Number of "High Beta" long straights (Xp=0)	16
Number of "Low Beta" long straights (Xp=0)	16
Beam Current (mA)	250
Bunch Length (at I=0) (ps)	22

Table 13

A Comparison Between the NSLS U/W Ring and the ESRF

Ports and Stations	U/W Ring	P-ESRF
A. BENDING MAGNETS		
λ_c (A)	0.86	2
Flux at λ_c/mrad (photons/mrad/1% BW)	2.3×10^{13}	2.7×10^{13}
Number of Ports	$\leq (32-N_{ws})$	10
mrad/port	10	10
B. MULTIPOLE WIGGLERS		
λ_c (A)	0.35	1
Flux at λ_c/mrad (photons/mrad/1% BW)	2.2×10^{15}	3.2×10^{14}
Number of Ports	N_w	38
mrad/port	2	2 (:2)
C. SHORT WIGGLERS		
λ_c (A)	0.09 to 0.35	0.25
Flux at λ_c/mrad (photons/mrad/1% BW)	8.8×10^{14}	2.7×10^{13}
Number of Ports	$\leq N_{ws}$	10
mrad/port	2	12 (:3)
D. UNDULATORS		
λ_1 (A)	0.86	
Number of Ports	$\leq (28-N_u)$	

Stanford University, SSRL--6-GeV-Ring Facility

SSRL has been studying new ring designs that are optimized around wiggler/undulator sources that give orders-of-magnitude-greater flux and brightness than bending magnets. SSRL experience with high-power wigglers reinforces the belief that, because of thermal problems, we are close to the limit of x-ray intensities that can be used at existing rings and that major advances in x-ray intensities and brightness require x-ray undulators that concentrate the spectrum in the desired region.

To utilize x-ray undulators effectively, high-energy storage rings (5 to 6 GeV) with very low emittance are required, along with a large number of straight sections for insertion devices. In the effort to achieve additional capabilities in the soft x-ray/VUV region, SSRL has studied the concept of having a 2-GeV ring with very long straight sections in the same housing as a 6-GeV ring. The rings would share the facility, thus reducing costs, and beamlines from each ring would alternate (spaced at six degrees) around the circumference.

Various designs for such a dual-ring system have been studied. A proposal and a conceptual design report for a 6-GeV facility are expected during 1984. The parameters now being considered are shown in Table 14.

Table 14

SSRL 6-GeV-Ring Parameters

Energy (GeV)	6
Circumference (meters)	532
Beam Emittance (m•rad)	5.7×10^{-9}
Beam Current	
per bunch (mA)	< 5.0
total (mA)	< 100
Beam Lifetime	
Touschek (h)	20
Coulomb Scattering (h)	20
Gas Bremstrahllung (h)	20
Total (h)	6.7
Bunch Length (ps)	~100
Average Vacuum (torr)	5.10^{-9}
SR Power (kW)	600
Insertions	
High Brightness	10
free length L(meters)	4
Small Spot Size	20
free length L(meters)	2

Some of the major design criteria beyond the need for a 6-GeV ring are:

- The beam current--both per bunch and total--should be moderate.
- The design should aim for the smallest reasonable beam emittance.
- In some insertions the brightness of the photon beams from an undulator should be maximized. This is achieved by reducing the beam divergence to such a level that the spectral line width as determined by the divergence is equivalent to the line width due to a 100-period undulator.
- There should be space for 30 insertion devices in the ring, and the aperture requirements for the beams should be minimized in both planes to allow short-period insertion devices to deflect the beam in either plane.
- The beam lifetime should be at least 10 hours.

These criteria are met with a new magnet-lattice arrangement using "triplett achromats" in between straight sections. This arrangement provides a small emittance and good flexibility and reduces the circumference of the ring by 30% for a given number of straight sections.

The radiation characteristics of the many possible sources in this ring are shown in Table 15.

Table 15

Radiation Characteristics of Possible SSRL 6-GeV-Ring Sources

High-Brightness Insertions	
Energy (GeV)	6
Beam Size σ_x/σ_y(μm)	324/116
Beam Divergence σ_x'/σ_y'(μrad)	13/13
Line width/γ (100 periods)	8.5×10^{-6}
Total Line Width/γ	2.0×10^{-5}
Minimum Gap G_x/G_y (mm)	7/5.5
Highest Fund Photon Energy εph(keV)	20
Small-Spot-Size Insertions	
Energy (GeV)	6
Beam Size $\sigma_x\sigma_y$(μm)	48/41
Beam Divergence σ_x'/σ_y'(μrad)	48/41
Minimum Gap G_x/G_y (mm)	2/2
Critical Photon Energy B_W = 20 kB ε_c(keV)	47.5
Bending Magnets	
Energy (GeV)	6
Bend Field (kG)	10.5
Critical Photon Energy (keV)	25

As in any high-energy ring with undulators and wigglers, a major design issue is handling the photon-beam power on downstream components in the beamline. The latest beamline at SPEAR (LBL/Exxon/SSRL 54-pole, 1.2-T wiggler) has front-end components designed to take power densities of 200 W/mm^2. Present downstream optical elements can take considerably less power density and many possible solutions are being considered. They include in-vacuum monochromators, new materials including multilayer and SiC mirrors, and 100-meter-long beamlines. With the assumption that power densities should not exceed twice the present level (i.e., $\leq$ 400 W/mm^2), SSRL has studied a wide range of undulator/wiggler parameters and has concluded that:

- An array of undulators can cover the energy range of from 3 to 21 keV in the fundamental, with conservative gaps and a source brightness of 10^{18} to 10^{19} photons/sec·mrad^2·0.1A·0.1%BW.
- Given the parameters of the 6-GeV ring, wigglers can operate with critical energies up to 40 keV.
- Continued research and development is required to improve the downstream optical components; much experience will be gained from the present high-power lines on SPEAR.

Summary of Future Facilities

It is clear from the above that future SR facilities will predominately use insertion devices and, as a result, will achieve source brightness that is orders of magnitude higher than would otherwise be possible. The storage-ring designs reflect this design direction in having small beam emittance and many insertions whose beam optics are tailored for undulators and wigglers. These trends are illustrated in Table 16, which gives a summary comparison of machine parameters and source characteristics for some representative existing and proposed SR facilities.

The ALS has been formally proposed for construction, and its projected performance and cost have been detailed above. This facility would enhance the US capability in the VUV and soft x-ray energy range.

In the harder x-ray range, there are several studies in progress, and proposals for construction are currently being initiated. These facilities will again use insertion-device-based storage rings but will operate at higher energies--around 5 to 6 GeV. Because injection at the operating energy is becoming increasingly important in optimizing the storage-ring design and in improving operation, it is worth noting that there are three locations in the USA where existing electron accelerators could be used as injectors, thereby reducing the construction cost of a high-energy facility. At Cornell studies have begun on a possible dedicated synchrotron light source that could use the high-energy-electron synchrotron as an injector. The cost of a 5 to 6-GeV facility including an injector is estimated to be approximately $168 million in FY85 dollars. This figure includes the experimental areas and an initial complement of approximately 10 undulator/wiggler beamlines. The designs could eventually accommodate 30 or more

Table 16

Storage-Ring and Device Parameters for Representative Facilities

		NSLS			SSRL	
	SPEAR (achieved)	VUV (achieved)	X-ray (design)	ALS (design)	PEP (design)	SSRL--6-GeV (design)
STORAGE RING						
Energy (GeV)	3	0.75	2.5	1.3 (1.9 max.)	15	6
Total current (mA)	100	300	500	400	20	100
Number of bunches	16	1	1 to 30	250	3	20 to 30
2σ bunch length (ps)	~ 200	400	330	23	70	200
Circumference (m)	234	50	170	182.4	2200	532
Horizontal Emittance (π-mrad)	4.5×10^{-7}	1×10^{-7}	1×10^{-7}	6.8×10^{-9}	1.2×10^{-7}	4.6×10^{-9}
Injection energy (GeV)	2.5	600 MeV	700 MeV	1.3	15	6
Number of bends	36	8	16	24	192	90
Number of quads	52	20	56	84	230	180
Number of straight sections for insertion devices	15	2	6	12	1[a]	30
Length of straight sections for insertion devices (m)	13 - 12m 2 - 5m	2.5	4.5	6	2[a]	10 - 4.3m (for undulators) 20 - 2.3m (for wigglers)
Beam lifetime (h)	15	1.5	8	8	8	6.7

TABLE CONTINUED ON NEXT PAGE

Table 16 (Continued)

Storage-Ring and Device Parameters for Representative Facilities

	SPEAR (achieved)	NSLS VUV (achieved)	NSLS X-ray (design)	ALS (design)	SSRL PEP (design)	SSRL--6-GeV (design)
PHOTON BEAMS						
--Bends						
Critical energy E_c (eV)	4700	430	5000	1230	4.5×10^4†	2.5×10^4
Photon flux at E_c for all ϕ (photons/s.mradθ·0.1% BW)	4.8×10^{12}	3×10^{12}	2×10^{13}	8.3×10^{12}	4.8×10^{12}†	9.6×10^{12}
--Wiggler						
Peak magnetic field (kG)	18	NR*	20	20	NR	8
Number of poles	8	NR	11	80	NR	20
Critical energy E_c (eV)	10,800	NR	8000	2250	NR	19,200
Photon flux at E_c for all ϕ (photons/s.mradθ·0.1% BW)	3.8×10^{13}	NR	2×10^{14}	6.7×10^{14}	NR	1.9×10^{14}
Total beam power (W)	3690	NR	8600	8560	NR	2900
Beam power density at 10 m (W/cm^2)	500	NR	5600	991	NR	8600§
--Undulator						
K factor	1	1	1	1	1	1
Full magnet gap (cm)	~ 3.5	1	0.7	1.2	5.8	0.8
Period length (cm)	6.1	2.6	2	2.67	7.5	2.06
Number of periods	30	96	150	187	26	200
First harmonic energy E_1(eV)	950	-	-	401	19,000	11,000
Spectral brilliance at E_1 (photons/s.mm^2·mrad^2·0.1% BW)	2×10^{15}	1×10^{17}	2×10^{17}	5×10^{18}	~ 9×10^{14}	3×10^{19}
Total beam power (W)	35	50	1700	344	115	2460
Beam power density at 10m (W/cm^2)	~ 600	110	4.1×10^4	930	1245	1.35×10^5
Beam power in central spot (W)	NR	0.7	800	9.3	NR	46

*One 2-m-long undulator is now in development for PEP. Future undulators could be 4 to 5-m long.
†Achieved
* NR = not relevant
§Front-end components would be located 25 m or more away from the source; power density drops quadratically with the distance from the source.

independently optimized beamlines. This estimate is comparable to that for the ESRF, which is in an advanced design stage.

In addition to the construction of new dedicated facilties, plans are underway to explore the physics opportunities of hard x-rays from undulators on existing high-energy storage rings such as PEP and CHESS. This effort raises the question of whether these facilities could be expanded as an alternative to the construction of a new ring. These storage rings were designed for colliding electron/positron beams, and their use for high-energy physics is expected to continue for many years. Parasitic or semidedicated operation of these rings for SR use is possible, but this would put severe technical limitations on the number and quality of insertion-device-based beamlines that could be made available. Even if one of these storage rings were to become available for dedicated SR use, their large beam emittance, their lack of provisions for installing insertions, and their location deep underground would make them a poor technical and economic choice as a basis for an advanced SR facility.

Cost Projections For Synchrotron-Facilities Development

Introduction

The committee had as its primary objective the establishment of priorities for the development of SR facilities in this country over the next decade. This development is to proceed through the utilization of the current generation of new machine, through the development of existing straight sections by means of insertion devices, and through the building of new, insertion-device-based machines.

The current generation of "new" synchrotron facility offers both increased brightness, due to better machine design, and added capability, due

to the expanded number of beamlines. There are also limited opportunities to develop and utilize insertion devices. The primary impact of this current generation of machine will be to:

1) make available a 10^2 to 10^4 increase in brightness, compared to previous machines, and

2) allow access by a wider community to the benefits of SR.

The increased beam quality achieved by these machines and the greater beam time they offer will allow expansion of ongoing studies and will cross the threshold for studies that were previously unfeasible. Intensified efforts at making these facilities "user friendly" will increase involvement by the materials-science and technology communities. Important research and development on beamline and endstation performance will be conducted to provide relatively low-cost gains in overall performance.

The development of insertion-device opportunities on existing machines will begin to establish the science possible with those devices and the technology applicable to the next-generation machine. Given the rapid movement in technology in this area, it is anticipated that there will be further advances over the near term. The revolutionary capabilities of these devices is expected to draw to the synchrotron area new communities of scientists and materials technologists, which will establish a new driving force for further capacity and expanded capability.

The construction of insertion-device-based machines, if implemented on the most expeditious schedule technically possible, cannot be expected to greatly impact the field until the late 1980s or early 1990s at best. The demand will then be high for insertion-device capability, as the emphasis is shifted to techniques requiring insertion-device performance.

Facility Cost Projections

There are three primary components to the facilities-development picture over the next 10 years: development of insertion-device capability on existing machines, design and construction of a high-energy facility to produce undulator radiation in the hard x-ray region, and construction of a low-energy facility to provide undulator capability in the soft x-ray ultraviolet (XUV) region. The individual development schedules for these components are as follows:

Development of Existing Straight Sections for Insertions -- There currently exists the following potential for new insertion-device development at dedicated facilities:

FACILITIES (USA)

Facility	Number of Straight Sections	Approximate Development Cost per Beamline (FY85 Millions of Dollars)
SSRL	4(short term)[a] 4(fully dedicated)	2.0 to 4.0
NSLS	7[b]	0.8 to 1.4
SRC	4	1.5

[a]One of these is included in SEPFF.
[b]Six are included for development in Phase II.

The actual development costs will of course depend to a great deal on the complexity of the beamlines involved. Their development should proceed at a measured pace to take advantage of technological advances, but at the same time user demand will force rapid development of a basic capacity.

The High-Energy Facility -- The high-energy facility is in the conceptual development stage. The design and engineering work needed to get to the proposal stage will take approximately two years. The construction-and-procurement phase will require approximately five years and has a projected cost of $168 million (in FY85 dollars), which can be broken down as follows:

Approximate Cost Breakdown for a 6-GeV Facility [a]
(In FY85 Millions of Dollars)

Engineering Design and Inspection	17
Conventional Construction	40
Technical Construction and Capital Equipment[b]	83
Contingency	28
TOTAL	168

[a]Cost figures provided by SSRL--figures are not reviewed
[b]Includes 10 instrumented beamlines and $14 million for an injector

The Low-Energy Facility -- The low-energy facility can be constructed from the existing ALS design at a cost of $72.6 million (in FY85 dollars). Construction will require four years. The cost is broken down as follows:

ALS Construction Costs
(In FY85 Millions of Dollars)

Accelerator Systems	30.5
Beamline Systems[a]	30.4
Conventional Facilities	11.7
TOTAL	72.6

[a]Includes 14 branch lines on 6 insertion-device ports

Users

Overview

The report on the "Current Status of Facilities Dedicated to the Production of Synchrotron Radiation" (the Lynch Report), published in 1983, concluded that user demand would saturate capacity by 1985. While the primary motivation for the actions recommended in this report is the creation of new opportunities in science and technology rather than the creation of added capacity, we found that indeed the Lynch Report projections seem to be valid. The NSLS XUV-ring bending-magnet ports are fully subscribed, and no more than four ports remain open on the XR ring. The SRC is approximately 70% committed even before becoming operational, and SSRL remains heavily oversubscribed. Development of the available straight sections by means of insertion devices is, of course, high among our recommendations, in concurrence with the Lynch report.

The following table shows, for the indicated years, the user count at various SR facilities and the number of publications arising from work done at each facility. The user count shown is the number of scientists who actually came to the facility to take data. Others associated with the proposals but not directly involved in data collection are not included. The user counts from 1983 are high in that they include the members of the NSLS x-ray PRTs who would have been at the facility had it been operational. NOTE: There is some overlap of users between the various facilities, in particular between NSLS and SSRL but between the others as well. This overlap is not accounted for in any manner.

	Users			Publications		
	1981	1982	1983	1981	1982	1983
SSRL	167	249	275	136	168	162
SRC	135	130	96	78	84	78
NSLS	-	-	398[a]	-	-	40
SURF	57	39	39	30	42	20
CHESS	15[b]	186	249	4	30	36[c]
TOTALS	374	604	1057	248	324	336

[a]Includes x-ray PRT members who would have been using the facility if it had been operating; 124 users actually took data on the VUV ring.
[b]Operation started in December 1981.
[c]70 more publications are presently in print.

A general idea of the SR-demand distribution across disciplinary boundaries can be obtained from the current breakdown of SSRL proposals, which is as follows:

Physical sciences	35%
Materials sciences	28%
Biology and medicine	21%
Chemical sciences	16%

User Interactions

SR facilities interact with a large number of users having various levels of expertise, under a variety of sometimes difficult circumstances. In order that efficient use be made of these limited and unique facilities, it is imperative that user interactions be carefully thought out and that facility personnel and users clearly understand their responsibilities and prerogatives. The classes of people involved in these interactions include facility managers, facility research personnel, facility technical personnel, scientific personnel from research groups that have built beamlines, users who have had extensive SR experience, and users who have had little or no SR experience. Furthermore, the users may need to operate under a variety of constraints ranging from the open research characteristic of university groups, to proprietary research having commercial restrictions, and to defense research requiring classification restrictions. The range of sociological interactions is large and complex. It takes effort and goodwill to assure that these facilities operate efficiently.

Dedicated SR sources operate 16 to 24 hours per day, seven days per week, for a large part of the year. The time scheduled for each user is highly variable, depending on the experimental requirements, and it is possible to have several user groups alternate in the use of a beamline during a day. Large research groups may have the manpower to operate for the required long hours, but small user groups and individuals require assistance. Such assistance might consist of cooperative interactions between small groups having common interests or interactions between the small user and a larger group. Cooperative research might also involve the user group and facility professionals, or the user group may arrange assistance from SR-facility technical personnel.

The SR-facility staff has responsibility for development of new instrumentation for the facility. Qualified user groups can greatly assist in this task. In fact, much of the advanced instrumentation at Tantalus, at SSRL, and at NSLS has been developed by user groups. Unfortunately, as facilities become larger and more complicated, sheer cost may prevent highly qualified university-based groups from developing beamlines. To assure continued participation by such groups, we urge that a sizable fraction (say 75%) of the beamlines at new facilities be developed by means of collaborations between such university groups and the facility staff. These collaborations would be similar to PRTs but with the important difference that funding would be provided by the instrumentation budget of the facility. Groups participating would be selected by a peer-review process to ensure their capability and suitability for the development proposed.

The policies that govern the use of beamlines will be developed by each facility to suit the local needs and conditions. In general, beamlines developed by the SR facility and by PRTs should be available to the general user community for a significant percent of the operating time. Beamlines developed by SR user groups other than PRTs should also be available to the general community for a part of the time. Even in the case in which a company develops a beamline at its own expense and pays "full cost" for the use of the beamline, use by the external community should be allowed and arranged through the SR-facility management. An exception to this cooperative-use arrangement may arise in the case of beamlines that are funded by the defense laboratories for classified work, but even in this case time should be available, given suitable controls.

The SR-facility management has the obligation to provide access on a "user friendly" basis. This obligation entails many things such as: adequate documentation of the facility equipment, along with assistance or instruction in developing the expertise to use it properly; adequate documentation for the required computer programs; controlled access to at least a limited range of support facilities and services such as storerooms, shops, office help, and darkrooms; and possibly other forms of assistance. While these forms vary, each SR-facility management has the obligation to facilitate the use of the beamlines. The "friendliness" of facilities is determined, in large part, by the helpfulness and cordiality of the staff with whom the users interact. It is exceedingly important, therefore, that such people be selected not only for their scientific or technical competence but also for their willingness to serve the user community. These qualities will be especially important in attracting future users from areas such as medicine and materials science. In general a "user committee" should exist to act as an intermediary between the user and the facility management when necessary. In addition to the above forms of assistance, it should be possible for the SR facility to help provide for housing and other amenities as deemed appropriate.

Scheduling of time on beamlines is a difficult and sensitive matter because the demand for usage is expected to exceed the available time. Again, only guidelines can be set down in view of the variety of beamlines and users. Scheduling procedures should be reviewed by the user committee. Proposals in the basic-science, applied-science, and technology categories should be judged on the basis of suitable standards in each category, and a balance should be sought between the three groups.

Research and Development

In order to develop the next-generation x-ray synchrotron facilities, a coherent long-range R&D plan must be implemented. The new SR facilities will be designed to incorporate a large number of undulators, which will provide for extreme-brightness, tunable radiation sources well into the hard x-ray region (15 to 20 keV), and wigglers, which will provide for photon energies into the 100-keV region. Such facilities will entail new problems in accelerator physics, in the development of undulator and wiggler sources, and in the handling of orders-of-magnitude-higher photon fluxes on beamline components such as monochromator crystals and grazing-incidence mirrors and gratings.

An overall plan, therefore, must address the following topics: (1) the development of science-driven goals for the performance of the machine, the insertion devices, and the beamline instrumentation, and (2) the implementation of appropriate R&D to assure successful achievement of these goals. Each of these topics is discussed below.

Development of Science-Driven Goals

This process is the scientific core of the development of SR facilities. It is by nature an evolutionary, community-wide process that is continually underway. We recommend that this process be fostered by the Department of Energy (DOE) sponsorship of periodic workshops to be held alternately at various laboratories. These workshops should be organized by a local committee of the host laboratory, working together with a national advisory group; the workshops should be international in scope. Travel budgets should be provided to encourage the attendance of the most experienced people and of those students and postdocs who are without adequate financial resources.

Indeed, one workshop has already been held at SSRL in June 1983, and another is planned for the summer of 1984. These workshops are endorsed by this committee provided that they involve international participation and that it is understood that the site chosen for such workshops will vary in the future. It is to the great benefit of the synchrotron community to encourage the participation of as many institutions as possible in the planning for next-generation sources. Further, it is our hope that a number of institutions will ultimately make proposals to construct the planned facility.

R&D Activities

Unlike the development of science-driven goals, the actual new-ring R&D activities pursued at each of the various institutions involved must be integrated with that institution's other R&D activities and must be commensurate with the talents and interests of the staff scientists at the institution. Such a process will necessarily involve some duplication of effort, but such duplication serves an essential function in scientific research and should not be considered wasteful. Both NSLS and SSRL have moved rapidly to develop R&D plans for FY 85 and FY 86 at the approximate level of $1.25M/year at each institution. We strongly recommend funding of these programs. The following summarizes the items that are considered important to address in these R&D plans; many of these items appear in the plans already developed.

Machine-Physics R&D

1. Multibunch instabilities
2. Ion trapping, measurements and calculations; the feasibility of the use of positron rings to alleviate ion trapping
3. Beam steering, orbit stability
4. Full-energy injection; utilization of a top-off mode to achieve "steady-state" operation

5. Vacuum studies (the vacuum is more important in low-emittance machines); desorption studies
6. Ring-lattice-structure studies, modular-prototype development
7. Development of new injector technology
8. New ring-control systems and beam diagnostics
9. Time-structure studies
10. Coupling of horizontal to vertical emittance.

Insertion-Device R&D

1. Calculation of photon fields from wigglers and undulators
2. Use of higher undulator harmonics
3. Minimum gap requirements
4. New methods of producing periodic magnet fields (e.g., the use of microwave devices)
5. Helical wigglers and other circularly polarizing devices
6. Permanent-magnet/hybrid-structure R&D, optimization studies, and in-vacuum devices
7. PEP undulators

Beamline-Instrumentation R&D

1. Beam-steering systems, detectors
2. Beryllium-window R&D, determination of thermal-stress limits
3. Thermal tolerances for optical elements; tests with simulated heating by lasers and electron beams
4. Mirror surfaces and effects of radiation, roughness, coatings, and metrology
5. Multilayer optics; focusing and monochromatizing
6. Ray tracing under thermally stressed conditions
7. Absolute-flux monitors
8. Optical observations of source image
9. Tests of cooling schemes (e.g., radiative cooling)

FACILITIES (USA)

10. Development of refractory x-ray optical elements, notably crystals for monochromators

11. Study of superficial contamination and desorption due to intense x-ray beams

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APPENDIX A

November 14, 1983 Letter to the Department of Energy

November 14, 1983

Dr. Alvin W. Trivelpiece
Director, Office of Energy Research
Department of Energy
Washington, D.C. 20585

Dear Al:

In this letter we will respond to your request to provide a status report on the Committee's deliberations on a long-range plan for advanced synchrotron radiation (SR) facilities in the U.S. We have met with over 75 scientists in Albuquerque on October 8 and 9, 1983, and in executive session at Stanford on October 26, 1983, and in Boston for two days on November 12 and 13, 1983. In this series of meetings we performed a critical review of both the scientific imperatives and facility options. We do not expect a final report until February 15, 1984. The great breadth and diversity of both the scientific and technological impact and facility options are the strength of SR. It is, therefore, a significant task to make sure all the opportunities and problems are correctly presented and documented in our final report. However, we can, at this time, provide you with an overview of the situation and a prioritized list of recommendations which we are certain will be featured in our final report.

OVERVIEW

The scientific and technological impact of synchrotron-based research is growing rapidly with numerous high quality advances in chemistry, biology, and physics, as well as in medical and materials technologies. As exciting as the past has been, the future opportunities in both science and technology are even greater. The new sources just being commissioned already offer a significant gain in capability from which new science will evolve. Insertion devices, which will form the basis of a revolutionary new generation of machines, promise such enormous gains in radiation flux and brightness that fundamentally new science can be approached.

There are significant plans already underway in Japan and Europe to exploit the new opportunities presented by insertion devices. Given the long lead time to develop these facilities, this country needs an aggressive program to provide such capabilities to our scientific and technological communities. The following recommendations represent such a program which we believe is justified by the scientific promise and practical importance of synchrotron radiation research.

RECOMMENDATIONS FOR A TEN-YEAR PLAN FOR SYNCHROTRON RADIATION FACILITIES AND SPECIFIC RECOMMENDATIONS FOR THE FY85 BUDGET CYCLE

The Committee recommends as its top priority that steps be taken to assure the timely completion of commissioning of NSLS and SRC as well as providing adequate operations budgets to assure the effective utilization of all existing facilities.

The future of synchrotron radiation research is clearly dependent on the significant gains offered by insertion devices. Our unanimous prioritized recommendations to exploit these new opportunities are as follows:

1) To realize the full potential of existing facilities, the Committee recommends expeditious completion of current projects to construct insertion device beamlines at SRC, NSLS and SSRL.

2) The Committee recommends the construction of a 6 GeV storage ring beginning in 1987 as a dedicated national facility. To achieve this objective, appropriate R&D funds must be allocated in FY85 and FY86.

3) The Committee recommends proceeding with the ALS in FY85 as a dedicated national facility.

The Committee strongly recommends that no action on a lower priority recommendation interfere with the timely pursuit of the higher priority items.

COMMENTS

The Committee determined that the physics of synchrotron radiation and insertion devices dictates different energy machines for the x-ray and XUV regions of the spectrum. The Committee unanimously concluded that if only a single new facility was to become available, the 6 GeV facility must have priority because it addresses regions of the spectrum and new science not accessible with insertion devices on existing dedicated facilities. In such an eventuality, the existing lower energy machines could be used to expand XUV insertion-based capability.

The difficulties presently being experienced in the commissioning of the newly constructed machines are not fundamental in nature and result partially from over-zealous attempts at economy. Therefore, our recommendations reflect the need for adequate funding for their commissioning and operations.

In our meetings and deliberations we received strong support for synchrotron radiation research from a broad spectrum of the scientific, industrial, and defense interests. We heard of achieved and potential breakthroughs in many areas, including catalysis, protein crystallography, angiography, plasma physics, and a broad spectrum of materials science.

There will clearly be considerable future growth in industrial participation as long as their participation is facilitated by user friendly instrumentation and the protection of their proprietary interests. The Committee also concluded that university participation would be greatly augmented if the funding for new beamlines at future and existing facilities was provided in such a way that outside groups can participate; and the facilities would profit greatly from their expertise. A proposal-based, peer reviewed approach for selection of outside participants is strongly recommended.

The rapid developments in synchrotron radiation led the Committee to unanimously recommend that a group such as ours be convened on not less than a yearly basis to review current developments in the entire field and to make recommendations for future actions.

While the Committee has considerable work still to do before completing its final report, we can already conclude that the aggressive program in synchrotron radiation that we have recommended will contribute significantly to the scientific, technological, and defense strength of this country.

For the Committee,

P. Eisenberger

M. L. Knotek

ADVANCED SYNCHROTRON RADIATION RESEARCH PLANNING STUDY

Committee Members

Peter Eisenberger, Co-Chairman - Exxon
Michael L. Knotek, Co-Chairman - Sandia
Charles Fadley - U. of Hawaii
E. Ward Plumer - U. of Pennsylvania
Dave Moncton - Brookhaven National Lab
Farrel Lytle - Boeing
Fred Brown - U. of Illinois
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Keith Hodgson - Stanford U.
Dave Nagel - Naval Research Lab
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Harry Gray - California Institute of Technology*
Dean Eastman - IBM
William Brinkman - Bell Labs
Guyford Stever - University Research Associates
Peter Wolff - Massachusetts Institute of Technology
J. E. Paterson - SLAC

*Illness prevented attendance

APPENDIX B

Survey of Synchrotron-Radiation Research Facilities Outside the USA

Introduction

Interest in synchrotron radiation (SR) research is growing so rapidly in many parts of the world that it is difficult to present an up-to-date comprehensive survey. This report attempts to briefly summarize the information that has been collected from numerous sources (questionnaires, laboratory reports, personal correspondence, etc.), with an emphasis on insertion devices and emittance, because these are of particular interest to the SR planning committee. The discussions of the different facilities vary greatly, reflecting the differences in the amount of information readily available.

In addition to providing a brief narrative about each facility (listed alphabetically by country), this appendix summarizes the available data in Table B-1 at the end of the appendix. More information, in the form of questionnaires filled out by individual laboratories, will be available in the proceedings of the 1983 U.S. National Conference on Synchrotron Radiation Instrumentation.

Also included at the end of this appendix are tabular summaries of European scientific interest (Table B-2) and of European storage-ring sources (Table B-3); these data are taken from the proceedings of the Scientific Worksohp held at Stanford in July, 1983 and are also available in "Synchrotron Radiation Facilities in Europe" by B. Buras, Y. Farge and D. J. Thompson, ESRP-PG-1/83, March, 1983.

Additional information on SR facilities is contained in the Lynch Committee Report ("Current Status of Facilities Dedicated to the Production of Synchrotron Radiation," available from the Solid State Sciences Committee, 2101 Constitution Ave., Washington, D.C. 20418) and in A. Bienenstock and H. Winick, "Synchrotron Radiation Research--An Overview," Physics Today, 36:48-58, June 1983.

Brazil

Feasibility studies are in progress that may lead to a proposal for a dedicated light source in the 1 to 3-GeV range.

China

Two facilities are under construction in the People's Republic of China. Both are scheduled to begin operation in about 1988. One is HESYRL, an 800-MeV, fully dedicated light source being built at the University of Science and Technology in Hefei, Anhui. The ring design follows the very successful approach of BESSY; it will have four configurations (general purpose, high flux, high brightness, and short pulse) and 24 ports from bending magnets and 3 from insertions. The injector is a 200-MeV linac that is extendable to higher energy. About 160 scientists are planning research at the facility.

The other facility is a partly dedicated 2.8-GeV ring BEPC in Beijing that will primarily be used for colliding-beam studies. Initially, a small parasitic SR research program was envisioned here, using two bending-magnet ports and two wiggler ports. The ring has four wigglers to control beam size for colliding-beam studies. Recently the design group has been asked to start over again in its design for the ring in order to provide for a larger SR program. The new lattice will have four additional insertions for SR purposes. A 1.1 to 1.4-GeV e^+/e^- linac is the injector. About 200 scientists are planning SR research at this facility.

England

The Synchrotron Radiation Source (SRS), a 2.0-GeV dedicated ring and the world's first multi-GeV ring to be designed and built as a radiation source, has been in operation since 1980 in Daresbury, England. The injector is a 600-MeV synchrotron.

A major program is now underway to upgrade the SRS through the construction of new facilities. The status of this program is summarized in the comprehensive appendix to the Daresbury Annual Report 1982/83, compiled by A. Jackson and K. R. Lea and available from Daresbury. According to this report, there are 27 experimental stations in operation or in construction, 10 of which were operational at the end of the 82/83 year and 4 of which are not independently operable. There are 236 scientists involved with 75 active proposals, plus 96 additional scientists involved with 63 exploratory agreements (which receive small amounts of beam time). A 5-T, 3-pole superconducting wiggler has begun operation. The wide fan from this device will ultimately be shared by seven independently operable stations. A permanent-magnet undulator is in construction.

Because of the increasing appreciation of the importance of beam brightness, a proposal has been made to modify the SRS to reduce the horizontal emittance from the present value of 150 to 11×10^{-8} m·rad. This modification will require a 5-month shutdown projected to start in September 1985.

Europe

For several years scientists from many western-European countries have considered various designs for an optimized hard x-ray source to be called the European Synchrotron Radiation Facility (ESRF). Early in 1983 an important step was taken toward the realization of this proposal with the establishment of the European Synchrotron Radiation Project, tentatively located at CERN in Geneva, Switzerland. The main task of this project is to prepare a site-independent proposal for the ESRF, discussing the scientific case, machine design, and instrumentation. At present the planning is for a 5-GeV ring with a full-energy synchrotron injector. The ring would have very low emittance ($E_x = 7 \times 10^{-9}$ m·rad) and it would accommodate 32 wiggler/undulator insertions. Site proposals have been made for the facility by RISØ, Daresbury, Trieste, Strasburg, and Dartmund; other site offers are expected. Progress is being made to secure the necessary multinational approvals, with authorization for construction expected by mid-1984.

France

In Orsay the LURE laboratory uses two operational rings and has one in construction. All rings use a 1.1-GeV e^+e^- linac for injection. The ACO 540-MeV ring is fully dedicated and has three bending-magnet ports serving 12 stations. Undulator/free-electron laser (FEL)/optical-klystron studies are pursued using one straight section. In 1983 the Orsay/Stanford group operated the first storage-ring FEL.

The DCI 1.72-GeV ring is used primarily for colliding-beam studies, with 25% of the beam time now dedicated to SR. In January, 1985 the DCI will become fully dedicated to SR. Two bending-magnet ports now serve 10 stations. An undulator and a superconducting wiggler are in construction. More than 350 scientists are involved with research at ACO and DCI and are planning research at Super-ACO.

Super-ACO, an 800-MeV dedicated source, is under construction and is scheduled for operation in late 1986. It will be a low-emittance ring (E_x = 3.0×10^{-8} m·rad) with six straight sections for insertions. Twenty-four bending-magnet stations are also planned.

A study is in progress for a 240 to 500-MeV permanent-magnet storage ring. In collaboration with the Lawrence Berkeley Laboratory (LBL), a prototype dipole and quadrupole are being built.

Germany

The major facilities here are BESSY, an 800-MeV dedicated ring in Berlin, and HASYLAB, which utilizes the 5.5-GeV ring DORIS in Hamburg in both dedicated (30%) and parasitic modes. Both rings have full-energy injectors. In addition, there are two synchrotrons (0.5 and 2.5 GeV) in Bonn that are used for SR.

BESSY has 22 stations in operation on bending-magnet beamlines and 6 more in construction. A multipole wiggler and undulator are under construction. Part of the facility is devoted to soft x-ray lithography by industrial groups, part is devoted to radiometry by the PTB (Physikalisch-Technische Bundesanstalt), and the largest part is devoted to use by the general scientific community. Three different magnet optics have so far been implemented: x-ray, metro (which has the lowest emittance), and ISO (which has a bunch length of 25 ps). A bunch length of 10 ps should be possible in the future. The BESSY group is planning a compact synchrotron source (COSY). It will be a 560-MeV ring with 5-T superconducting bending magnets and a 38-cm radius of curvature. About 56 scientists are active in research at BESSY, excluding students and postdoctorates.

HASYLAB has 28 bending-magnet experimental stations in operation and more in construction. A multipole wiggler is being built. Four hundred scientists from more than 80 institutions are involved with SR research at HAYSLAB, and there are others associated with the European Molecular Biology Laboratory outstation on DORIS. The annual HAYSLAB Activity Reports contain much detailed information about the lab and its program.

India

The Indian government has approved in principal the construction of SR research facilities. Several design approaches are being considered.

Italy

The PULS project utilizes the ADONE 1.5-GeV ring in both dedicated and parasitic modes. Four bending-magnet stations, two wiggler stations, and one undulator station are in operation. More wiggler stations are under construction. Injection is from a linac at 300 MeV. About 200 scientists use the facility each year.

Japan

Four fully dedicated storage rings are now in operation, one dedicated ring is proposed, and two colliding-beam rings that will also be used for SR are under construction. In addition, a 1.3-GeV synchrotron is used for SR.

The main facility is the Photon Factory, a 2.5-GeV fully dedicated ring that has been in operation since 1982. Injection is at full energy from a linac. In operation are 19 experimental stations on bending-magnet lines, 4 on a superconducting wiggler line, and one on a permanent-magnet undulator line. The superconducting wiggler is unique in having a horizontal field and hence in producing a vertically polarized beam. The Photon Factory is located at the KEK Laboratory, which has two colliding-beam rings in progress. These rings will also be used parasitically for SR. The Accumulator ring (6 GeV) began operation in November, 1983, and the Tristan main ring (30 GeV) is under construction. Future plans include low-energy rings along the 2.5-GeV linac. Six hundred scientists are now involved in performing or planning research at the Photon Factory.

The TERAS 600-MeV dedicated ring has been in operation at the Electrotechnical Laboratories in Tsukuba since 1982. It is used for lithography, radiometry, and other vacuum ultraviolet (VUV) studies. Injection is at 300 MeV from a linac.

The 380-MeV SOR ring at the Institute of Nuclear Science (INS) of the University of Tokyo is the first ring to be designed and built as a dedicated light source. Injection is at 300 MeV from the INS 1.3-GeV synchrotron. The storage ring began operation in 1974. The SOR ring program is under the direction of the Institute for Solid State Physics (ISSP) of the University of Tokyo. Five stations use bending-magnet radiation. A permanent-magnet undulator was tested in this ring, but limited experimental space precludes full utilization of such insertions. The ISSP group has proposed a new source, Super SOR, a 1.0-GeV low-emittance ring with eight long straight sections for insertions. This ring is described in the proceedings of the 1983 International Conference on High-Energy Accelerators (to be published).

At the Institute of Molecular Science in Okazaki, the first stored beam was obtained in November, 1983 in the 600-MeV UVSOR ring. Eleven experimental stations are under construction. The ring can accommodate four insertion devices. Injection is from a 600-MeV synchrotron. Two hundred scientists are planning research at this facility.

Sweden

The MAX 550-MeV storage ring/pulse stretcher is under construction at Lund. The facility will be shared by SR and nuclear-physics users. Four experimental stations are under construction.

Taiwan

The Taiwan Light Source (TLS), a 1-GeV low-emittance ring is approved for construction by the government and is now in design. Five straight sections will be available for insertions. It will be located near universities in an industrial park in Hsin Chu, about 50 miles from Taipei. About 100 Taiwanese scientists are planning to do research at the facility.

USSR

The main SR facilities here are at the Institute of Nuclear Physics in Novosibirsk, Siberia, which operates three storage rings, VEPP-2M, VEPP-3, and VEPP-4, all of which were built as colliding-beam rings. VEPP-2M is now largely used as a dedicated VUV/soft x-ray source, with eight experimental stations in use. This ring has an operational helical undulator originally built for high-energy-physics purposes but also useful as a source of circularly polarized radiation.

VEPP-3 supports a major program of x-ray research on its experimental stations. Much work has been done on VEPP-3 with insertion devices, including a 3.5-T, 20-pole superconducting wiggler and permanent-magnet undulators used primarily for optical-klystron experiments. Although VEPP-3 is not itself used for high-energy-physics experiments, it is part of the injection system for VEPP-4 and therefore only available for SR research for about 6 weeks per year.

VEPP-4 is a powerful x-ray source that is being fitted with beamlines, insertion devices, and experimental stations, of which some may already be in operation.

The Novosibirsk group has designed and built a 450-MeV storage ring that is being set up as a dedicated source at the Kurchatov Institute in Moscow. This ring will also be the injector to a proposed 2.5-GeV dedicated SR source.

A small 100-MeV storage ring, the N-100, has been operational at the Karkhov Physics Institute for many years.

Table 8-1

STORAGE RING SOURCES OF SYNCHROTRON RADIATION

H. WINICK
JANUARY 1984

Location	Ring	Gev	Emittance[a] (10^{-9} p m-rad)	Exp.[b] Stations	Insertion[c] Devices	Status/ Use
BRAZIL						F.S./Ded
CHINA						
Beijing	BEPC	2.8	66(18)		8	C/PDed
Hefei	HESYRL	0.8	9(1.3)		3	C/Ded
ENGLAND						
Daresbury	SRS	2.0	150 (11)		1 (4)	Op/Ded
EUROPE (T.B.D.)[d]	ESRP	5	0.7		30	P/Ded
FRANCE						
Orsay	ACO	0.54	15	12	1	Op/Ded
	DCI	1.8	150	10	2 (3)	Op/PDed[e]
	Super ACO	0.8	3		6	C/Ded
GERMANY						
Hamburg	DORIS	3.7-5.5	27	30	1 (4)	Op/PDed
W. Berlin	BESSY	0.8	4(2)	28	1(2)	Op/Ded
	COSY	0.56	250	8	-	C/Ded
INDIA						
Poona		1.5				P/Ded
ITALY						
Frascati	ADONE	1.5	22.5	6	2(3-4)	Op/PDed
JAPAN						
Okasaki	UVSOR	0.6	8(3.3)	11	2(4)	Op/Ded
Tokyo	SOR	0.38	30	5	1	Op/Ded
	Super SOR	1.0	2.0		8	P/Ded
Tsukuba (KEK)	Photon Factory	2.5	50(15)	24	2(7)	Op/Ded
	Accumulator	6-8	48		3	C/Par
	Tristan	30	18		0	C/Par
Tsukuba (ETL)	TERAS	0.6				Op/Ded
SWEDEN						
Lund	MAX	0.55	3	4	(2)	C/PDed
TAIWAN						
Hsin Chu	TLS	1.0	4		5	P/Ded
U.S.A.						
Berkeley	ALS	1.3	.68		12	P/Ded
Gaithersberg	SURF	0.28	27	11	-	Op/Ded
Ithaca	CESR	5.5	30(4)	8	1(3)	Op/Par
	New Ring	5-6				P/Ded
Stanford	SPEAR	3-4	45 (13)	19	4 (12)	Op/PDed
	PEP	15.0	15 (3)	1	1	C/Par
	SXRL	1.0	1.0		4	C/PDed
	New Ring	4.0	0.46		30	P/Ded
Stoughton	Tantalus	0.24	33	11	(2)	Op/Ded
	Aladdin	.75-1.0	(6.3)	19	(3)	Op/Ded
Upton	NSLS-I	0.75	13(9)	33	2	Op/Ded
	NSLS-II	2.5	(8)	32	4(5)	Op/Ded
	New Ring	6.0	0.7		32	P/Ded
USSR						
Harkhov	U-100	0.1				Op/Ded
Moscow	Kurchatov-I	0.45				C/Ded
	Kurchatov-II	2.5				P/Ded
Novosibirsk	VEPP-2M	0.7		8	2	Op/PDed
	VEPP-3	2.2		9	2	Op/PDed
	VEPP-4	5-7		6	2	Op/Par

(a) Emittance: For operational rings the lowest achieved horizontal emittance is given. When a range of operation energies is given the quoted emittance is at the lowest electron energy. Emittance scales as the square of electron energy. ( ) indicates planned or possible future value. For rings not yet in operation the lowest design emittance is given.

(b) Experimental Stations: The total number of stations in operation or in construction in 1983 is given.

(c) Insertion Devices: For operational rings the number of insertion devices in use and in construction is given. ( ) indicates maximum number possible. For rings not yet in operation the number given is the maximum possible number.

(d) T.B.D. - to be determined

(e) The DCI will be fully dedicated in January 1985.

F.S. = Feasibility study
Op = in operation
Ded = dedicated
P = Proposed
PDed = Partly dedicated
C = In construction
Par = parasitic

Table B-2

European Interest in Synchrotron Radiation Research (based on answers to a recent (1982) questionnaire)				
Number of groups (number of scientists)				
Country	Interested in S.R.	Have experience in S.R.	Indicated problems	Made concrete proposals
Austria	7 (44)	3 (14)	3 (16)	3 (23)
Belgium	31 (214)	9 (71)	12 (112)	7 (62)
Denmark	14 (28)	3 (10)	3 (10)	3 (10)
Finland	11 (47)	6 (27)	5 (22)	4 (19)
France	145 (643)	89 (422)	93 (449)	77 (376)
Germany	82 (551)	53 (349)	41 (252)	26 (181)
Great Britain	57 (192)	43 (145)	33 (135)	26 (97)
Netherlands	2 (70)	1 (35)		
Norway	6 (27)	3 (8)		
Italy	83 (236)	54 (150)	26 (73)	19 (71)
Sweden	17 (86)	4 (16)	11 (54)	6 (29)
Total	455(2138)	268(1247)	227(1123)	171(868)

Table B-3

Storage Rings in Europe Emitting S.R.

Name Location	Electron GeV	Electron mA	Photon keV ε_c	Number of Stations	W[x], U[x] FEL[x]
ACO Orsay	0.54	150	0.31	15	U for FEL
MAX[+] Lund	0.55	(200)[+]	0.31	0(3)	
BESSY Berlin	0.8	200 (500)[+]	0.62	22	(W,FEL)
Super ACO[*] Orsay	0.8		0.65		(7U)
ADONE Frascati	1.5	≤100	1.5	4(5)	W, FEL
SRS Daresbury	2.0	280 (370)[+]	3.2	8(27)	1W (1W)
DCI Orsay	1.8	300	3.4	7	(1-3W)
DORIS Hamburg	3.5- -5.6	30- -200	22.9	25	(1)
PETRA[**] Hamburg	18.0	20	67.4	0	

x) See text; in parenthesis the number of devices under construction.

+) Expected values.

*) Under construction.

**) Not used for S.R. research

APPENDIX C

Alternate Photon Sources

Laser Sources

Several groups have used nonlinear optical techniques to produce vacuum ultraviolet (VUV) and soft x-ray ultraviolet (XUV) pulses.[1] The shortest wavelength achieved to date, via seventh-harmonic generation in He gas, is 355 A.[2] There has also recently been a report of a 930-A stimulated emission in krypton gas.[3] These experiments all require powerful pump lasers ands complicated vacuum and gas-handling systems. Nevertheless, the equipment costs are modest compared to those of an ultraviolet (UV) synchrotron. Thus, it is pertinent to ask how laser UV sources might, in the future, compete with synchrotron UV sources.

Laser UV sources generally make use of high-order optical nonlinearities and require intense pump beams. They inevitably operate in a pulsed mode with relatively low repetition rate (10 Hz is typical). The average power generated by such devices is orders of magnitude lower than that of a UV synchrotron. Hence, for conventional, continuous-wave (CW) spectroscopy, the synchrotron will almost always be superior to a laser source. At present, most UV spectroscopy is CW spectroscopy.

Looking to the future, however, one can envisage a growing need for short, intense UV pulses. A number of biological and chemical-kinetics experiments require UV pulses in the nanosecond range; for other chemical applications and for many time-resolved condensed-matter-science measurements, picosecond pulses are needed.

The bunch structure of synchrotron beams naturally generates pulses in the 0.1 to 1.0-ns range, but it will be difficult to produce bunches shorter than 20 ps. Thus, direct picosecond spectroscopy with synchrotrons does not seem feasible. It has been suggested that picosecond time resolution might be achieved, in an indirect way, by making use of the extreme reproducibility (in shape and time) of the synchrotron pulses.[4] That technique, termed Harmonic Phase-Shift Analysis, has recently been demonstrated at the picosecond level. Laser UV sources, on the other hand, often generate pulses in the picosecond range and could be modified, without excessive difficulty, to produce subpicosecond pulses with some degree of tunability. Thus, it can be argued that the laser source, rather than the synchrotron, is the natural tool for picosecond UV spectroscopy. A number of scientists hold that view, and several excellent groups in the U.S. are trying to develop pulsed UV sources for such purposes.

Until recently, laser sources for the XUV required complicated differential-pumping systems. The nonlinear process generating the radiation takes place in a moderately dense gas, whereas high vacuum is needed for subsequent experimentation. This difficulty has now been eliminated in systems employing pulsed supersonic jets. Though still inefficient, these devices promise ultimately to produce sufficient energy for such experiments as time-resolved XUV photoemission.

Facilities for generating XUV picosecond pulses via laser techniques will cost on the order of $1M; though not inexpensive, the price is small compared to that of a synchrotron. At this stage, it is not clear that either laser sources or synchrotron sources can actually be used for picosecond UV spectroscopy. The current vigorous research effort on laser-produced XUV pulses should soon determine the potential of that technique. To date, there has not been a comparable experimental program concerning the use of synchrotron-generated UV pulses to achieve picosecond time resolution. Such measurements would be valuable; if successful, they would strengthen the case for constructing the Advanced Light Source (ALS). At present, however, the claim that ALS will be capable of doing subpicosecond UV spectroscopy is largely based on theoretical ideas that have not been extensively tested and that are viewed with some skepticism in the picosecond-optics community.

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5. Physics Today, November 1983, page 19.

Plasma XUV Sources

Multimillion-degree plasmas emit intensely in the extreme UV and soft x-ray regions ($\lambda > 3$ A). Hence, they are useful in the range below 1000 eV where operation of coherent direct-laser or harmonic-generation sources is not yet routine. Intensities available from plasma sources make them useful alternatives to synchrotron radiation (SR) for some experiments and superior to current storage-ring sources for other measurements.

Hot, dense laboratory plasmas of use as XUV sources are never large enough to be optically thick. That is, they are not blackbody radiators at short wavelengths. Their spectra consist of numerous lines on top of usually much weaker continua from recombination and Bremsstrahlung. At wavelengths longer than about 30 A, the lines can be so dense that plasma-emission spectra from high-atomic-number elements are effectively continua. Plasmas that are dense enough to emit x-rays intensely are commonly about 1 mm in extent. They produce x-radiation for times usually in the 100-ps to 100-ns range, depending on

the method of plasma heating. XUV radiation from plasmas is unpolarized, incoherent, and emitted into large solid angles (>2π sr). Laboratory plasma XUV sources now typically cost $200K to 400K.

Two types of energy sources are employed to produce x-ray hot plasmas--lasers and electrical discharges.[1] Laser wavelengths in or near the 1 to 0.1-μm range are of most interest. Nd systems (1.06 μm, with harmonics at 0.53 and 0.35 μm) and excimer lasers at 0.31 or 0.25 μm have been or soon will be used for plasma XUV-source work. Capacitor banks, used either alone or with a pulse-forming network, are employed to produce electrical discharges greater than 100 kA that heat plasmas resistively or by magnetic-field-driven implosions. No matter how heated, plasma x-ray sources involve undesirable vapor (the expanding plasma) and sometimes debris. That is, they are not as clean as storage-ring sources.

X-rays from plasmas produced by very large, low-repetition-rate (10^{-3} Hz) Nd lasers have been widely measured in fusion-research programs for the past decade. Wavelengths as short as 0.1 A have been recorded. Now XUV radiation down to 1 A, produced by table-top Nd and excimer lasers that operate at 10 to 100 Hz, is being measured. Uses of soft x-ray emission from laser-heated plasmas are now increasing rapidly. The formation was announced recently of a U.S. company that will sell a lithography system using x-rays from laser-heated plasmas. Development of 100-W slab-glass Nd and excimer laser systems engineered for optimum production of x-ray-emitting plasmas is in progress. Such systems may be commerically available in a few years. Lasers for x-ray generation must have both high peak power (short energetic pulses), to achieve plasma temperatures adequate for efficient x-ray emission, and high average power (high repetition rate), to yield high average x-ray power.

Absorption of laser radiation by a target typically varies from about 50% with Nd at 1.06 μm to over 75% for excimer-laser wavelengths near 0.25 μm. As much as 30% of the incident laser energy can be emitted as XUV radiation in the 3 to 300-A region. Conversion efficiencies depend on target and focal conditions as well as on the laser-pulse characteristics. For some conditions, up to 0.1% of the incident laser energy can be re-emitted in a single strong x-ray line. XUV radiation from laser-heated plasmas mostly arises from a region less than 1 mm in diameter. In the 1 to 10-ns range, XUV pulse lengths are comparable to the laser pulse length. For picosecond lasers, plasma cooling extends x-ray emission times, so that x-ray pulses much shorter than 100 ps are uncommon. The limit on laser plasma x-ray emission times may be near 10 ps.

X-rays from large terawatt electrical-pulse generators have also been studied for the past ten years in fusion and weapons-related programs. Now, smaller, 10 to 100-MW pulsed-power systems are available commercially to produce x-ray-emitting plasmas at rates near 10^{-1} Hz. Their use is lagging the employment of lasers as plasma x-radiation sources because laser technology is more widely known and because laser systems tend to have more uses.

Materials for the plasmas in discharge-heated x-ray sources can originate from four different sources: 1) solid material (e.g., fine wires) placed across the interelectrode gap, 2) low-pressure gas filling the interelectrode region, 3) gas puffed into the cathode/anode gap immediately prior to the discharge, and 4) erosion of the electrodes. Of these, the puff sources are most reproducible, easiest to operate, and have the best chance of operation at rates exceeding

1 Hz. Whereas a laser-heated plasma will currently produce only 100 mJ of XUV radiation at 10 Hz (1 watt), commerical puff sources now yield about 20 joules at 10^{-1} Hz (2 watts). The line spectra from the puff source falls in the 4 to 40-A range, depending on the gas used, while x-radiation from CW laser plasmas tends to fall near 20 A. X-ray emission from discharge-heated plasmas is most intense from a cylindrical region about 1 mm in diameter and 1 cm long, with emission times of 10 to 100 ns.

Detailed comparisons of the radiation from plasma XUV sources with direct laser emission or SR are complex and can only be done on a case-by-case basis.[2] The wide variation in geometry among the different sources (e.g., emission directions) tends to require the use of different monochromators with different sources. However, in general, plasma sources of XUV radiation are superior to storage rings for peak power, and the opposite is true for average power. Some dynamic measurements, such as flash x-ray diffraction from or radiography of rapid events, require high peak intensities. Nonlinear x-ray-optics experiments that require high peak x-ray intensities are expected. Calibration of instrumentation for pulsed-x-ray measurements is also done with plasma radiation. Uses of laser plasma x-radiation in atomic, molecular, and solid state (surface) studies were examined recently, and many of them apply to discharge-heated sources also.[3]

In general, the development and use of plasma XUV sources is now where employments of SR sources was 10 to 15 years ago. Devices, especially lasers, that were engineered for other uses are being applied to x-ray generation, a process that is the equivalent of parasitic SR usage. However, lasers and discharge sources specifically designed for x-ray work are becoming increasingly available, and these items are analogous to dedicated storage rings. Plasma x-ray sources will not supplant storage rings. They may, however, be widely available for a variety of work within the next decade.

1. For recent review of plasma x-ray sources oriented toward x-ray lithography, see D. J. Nagel in N. G. Einspruch (Editor) VLSI Electronics, Volume 7, Plasma Processing for VLSI, Academic Press, New York (1984) p. 137.

2. E.-E. Koch (Editor) Handbook on Synchrotron Radiation, Vol. 1A, North-Holland, Amsterdam (1983) p. 41.

3. D. J. Nagel, "Characteristics and Uses of X-Radiation from Laser-Heated Plasmas," Society for Photographic Instrumentation, Vol. 447 (1984).

Free-Electron Laser (FEL) Sources

In the language of this report, the radiation provided by an FEL is stimulated undulator radiation. The first observation of FEL behavior was made in the early 1970s by Madey and coworkers on the Stanford superconducting linear accelerator. Since that time there has been a rush of activity. Using laboratory-scale accelerators (approximately 10 MeV), groups at Santa Barbara (funded by the Air Force) and at Bell Laboratories are exploring the use of FEL sources in the far infrared (75 μm to 2 mm) region. Other groups, at

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the National Synchrotron Light Source (NSLS) on the 750-MeV storage ring and in a joint Stanford/LURE project in France, have been pursuing FEL operation in the visible region, with the goal of ultimately moving into the UV and XUV regions. These storage-ring applications use insertion devices that are very similar to the ones described in this report but that have first harmonics in the visible region. The Stanford/LURE collaboration has successfully observed lasing action in the visible (red). While attempts at NSLS continue, Madey has obtained Department of Defense (DOD) funding to build a 1-GeV storage ring for FEL studies; the plans are to push the wavelength into the UV and XUV region and to increase the power in the visible. Because of the damage to mirrors by the accompanying x-ray SR, there are serious problems in going to the UV.

Calculations of the power and brightness of the radiation produced by storage-ring-based FELs are very impressive, and this radiation will certainly be more intense and brighter than the SR that can be produced in the UV. Thus, the net impact of FEL sources will significantly depend on how far into the XUV they can successfully achieve lasing.

Other concepts such as the transverse optical klystron also offer opportunities for producing UV laser radiation. It is unlikely that they will go above 100 eV. The storage ring designed for FEL use obviously can produce SR in the XUV region and as such is both complementary and supplementary to other activities. At Stanford, for example, the SR and FEL programs will share the new ring that is being built primarily for FEL development.

Because of the FEL's similarity to insertion devices, calling it an alternative source rather than another use of insertion devices in a storage ring is somewhat questionable. In any case, the development of FELs should certainly be pursued in both the infrared and the UV; their development is of course of great interest to the SR community. Hopefully, the new facility at Stanford will be made available as appropriate to the SR community.

1181

Major Facilities for Materials Research and Related Disciplines

Major Materials Facilities Committee
Commission on Physical Sciences, Mathematics, and Resources
National Research Council

NATIONAL ACADEMY PRESS
Washington, DC 1984

NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the committee responsible for the report were chosen for their special competences and with regard for appropriate balance.

This report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

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Support for this project was provided by the Department of Energy under Grant No. DE-FG01-84ER45062 and by the National Science Foundation under Grant No. DMR-8408982.

Available from
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Commission on Physical Sciences,
Mathematics, and Resources
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NATIONAL RESEARCH COUNCIL

2101 CONSTITUTION AVENUE WASHINGTON, D. C. 20418

OFFICE OF THE CHAIRMAN

July 24, 1984

Dr. George J. Keyworth, III
Director
Office of Science and Technology
Policy
Old Executive Office Building
Washington, D.C. 20500

Dear Jay:

I am pleased to transmit a report on major materials facilities, prepared at your request by a committee of the National Research Council (NRC). As with all reports of the NRC, the report is the responsibility of its committee, but its review has been monitored by the Academies' Report Review Committee.

The report presents priorities both for new facilities and new capabilities at existing facilities with initial cost of at least $5 million. The new facilities in order of priority are: a 6 GeV Synchrotron Radiation Facility; an Advanced Steady State Neutron Facility; a 1 to 2 GeV Synchrotron Radiation Facility; and a High Intensity Pulsed Neutron Facility. The new capabilities at existing facilities in order of priority are: centers for cold neutron research, incorporating guide halls and instrumentation; insertion devices on existing synchrotron radiation facilities; an experimental hall and instrumentation at the Los Alamos National Laboratory Pulsed Neutron Source; upgrading of the National Magnet Laboratory; and enriched pulsed neutron targets.

The context for these recommended priorities is given in the executive summary, and more fully set out in the three chapters of the report proper. Chapter I titled, Materials Research: Facilities and Modes, describes the nature of materials research, by whom it is done, and for what purposes; and the major facilities for synchrotron radiation, neutron scattering, and high magnetic field research, in the United States

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and other countries. Chapter II titled, Major Materials Facilities: Science and Technology, outlines the research that has been done with existing facilities and that will be facilitated with the proposed new installations. Chapter III titled, Conclusions and Recommendations, offers a fuller rationale for the priorities, briefly analyzes costs, and surveys facilities considered but not included in the priorities by virtue of the Committee's charter and without necessarily passing any judgment on their relative merit.

As acknowledged in the preface to the Report, setting priorities was a "difficult and painful" task for the Committee. It should be understood that, in accordance with your request, the report did not address the question of balance between support for "small" and "big" science in materials research. The Committee hewed to its charter: to set priorities among major facilities considered important to the nation's research efforts. Therefore, the report should not be read as advocating increased support for major facilities to the detriment of smaller scale science, typically done at universities, governmental laboratories, or regional centers. Indeed, quoting from the preface, "additional panels should be convened to address other aspects of materials research and to review previous recommendations in light of new information."

With those caveats in mind, I believe this report to be a major contribution to guiding the science and technology of the United States. All of us understood that selecting priorities is a difficult task. That it was done, with care and wisdom, is due to the members of the committee, to its staff, and to the Committee's leaders, Frederick Seitz and Dean Eastman.

I commend the report to your attention.

Sincerely,

Frank

Frank Press
President

Attachment

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PREFACE

The President's Office of Science and Technology Policy in November 1983 asked the National Research Council (NRC) to assist in establishing priorities for major facilities for materials research. These facilities, defined as those with initial cost of at least $5 million, include, among others, sources of synchrotron radiation and steady state and pulsed neutrons.

A committee of twenty-two members was formed within the NRC Commission on Physical Sciences, Mathematics, and Resources, representing the diverse disciplines that use facilities for major materials. The Committee's membership was also intended to mirror the differing research styles and the spectrum of organizations where the research is done. Scientific work with materials varies from that principally requiring laboratory-scale instrumentation to that dependent on the availability of major facilities that the Committee was asked to address. It is done by governmental, academic, and industrial scientists and engineers.

The Major Materials Facilities Committee first met late in January 1984 and three times thereafter. Four panels of the Committee were formed: three to consider and make recommendations to the Committee regarding needs for synchrotron radiation, neutron scattering, and other specialized materials research facilities; and a fourth to analyze the budgetary implications of various sets of priorities. During its tenure, the Committee, or one of its panels meeting separately, was informed of or heard detailed presentations on the status and promise of many of the U.S. major materials facilities falling within its charge. Further, the President's Science Advisor, the directors of several national laboratories, and senior research officials of several federal agencies met with the Committee. [A list of presentations to the Committee is in Appendix C.] Finally, the Committee had available to it recently completed and advance drafts of reports relating to its topic, done by the National Research Council, the Department of Energy, and other organizations. In all, this report is the result of more than 6 months of extremely intensive efforts by the Committee, its panels, and its staff.

In addition to the executive summary, the report contains three chapters. Chapter I describes the facilities, research styles, and research performers of materials research in the United States. It

also offers a brief summary of the status of U.S. facilities vis-a-vis those of other countries. Chapter II outlines scientific and technological accomplishments using major materials facilities and suggests the likely direction of future research. In short, it presents the scientific and technological rationale for the recommendations in this report. Chapter III expands on the conclusions and recommendations given in the executive summary.

A continuing concern throughout the Committee's deliberations was the possible misinterpretation, even misuse, of its report. As is emphasized several times in the text that follows, the knowledge generated by materials research comes from diverse research styles and performers, each vital to the total effort and each complementary to the other. These varying styles must each be well supported, for the health of the total effort in materials research. To deny funding to smaller scale research to support major facilities is destructive. Therefore, the recommendations in this report should be read and interpreted for what they are: a statement as to priorities solely for major materials facilities. The Committee did not address, and this report does not imply, any judgments on the total spectrum of work embraced by materials research.

By the same token, additional panels should be convened to address other aspects of materials research and to review previous recommendations in light of new information. Such panels, by responding to specific aspects of materials research needs, can contribute to the long-range planning and to the setting of priorities for the materials research field.

The task before the Committee was difficult and painful. Its recommendations, and its omissions, would, if they were adopted, have a major effect on the future direction of materials research in the United States, on the institutions where major facilities are or may be based, and, likely, on the future competitive status of major segments of United States technology. That the Committee fully agreed to the need to recommend priorities testifies to the cosmopolitan views of its members; that reaching agreement on priorities was difficult testifies to their strong beliefs in the value of particular facilities.

The National Research Council is indebted to the members of the Committee for their patience, goodwill, and dedication to an arduous and trying task.

Dean E. Eastman
Frederick Seitz
Co-Chairmen, Major Materials
Facilities Committee

CONTENTS

	PREFACE	xi
	EXECUTIVE SUMMARY	1
	Conclusions and Recommendations	3
	Recommended Priorities	3
I.	MATERIALS RESEARCH: FACILITIES AND MODES	7
	Universities	7
	Federal Laboratories	10
	Industry	10
	Major Materials Facilities	11
II.	MAJOR MATERIALS FACILITIES: SCIENCE AND TECHNOLOGY	17
	Synchrotron Radiation, Neutron Scattering, and Magnetic Fields	17
	Synchrotron Radiation Research: Past and Future	21
	Neutron Scattering Research: Past and Future	30
	Research with Magnet Facilities: Past and Future	37
	Advanced Technology Needs: Applications of New Facilities	40
III.	CONCLUSIONS AND RECOMMENDATIONS	43
	Recommended Priorities	44
	Estimated Costs of the Recommendations	49
	Other Specialized Facilities Considered by the Committee	54

APPENDIXES

A.	REPRINT: George H. Vineyard and L. M. Falicov, "National Facilities for Research in the Physics of Condensed Matter," Review of Scientific Instruments, Vol. 55, No. 4, 620-630, April 1984	57
B.	REFERENCES AND RELATED LITERATURE	69
C.	LIST OF PRESENTATIONS MADE TO THE MAJOR MATERIALS FACILITIES COMMITTEE (the complete presentations will appear in a supplement to this report)	73
D.	PRESENTATIONS TO PANELS	77

EXECUTIVE SUMMARY

The science of condensed matter, or materials research, deals with the properties of solids and liquids and their interfaces. It is interdisciplinary, involving materials science, major areas of physics and chemistry, and the earth sciences, biology, and medicine. The understanding of the behavior and properties of materials undergirds every major technology; as a consequence, strength in materials research is essential to national capacities in advanced technology and, hence, to economic competitiveness.

Like all sciences, materials research depends on instruments, with these instruments ranging from laboratory size, such as mass spectrometers, to major national facilities, such as sources of synchrotron radiation and neutrons.

This report deals solely with major facilities. That was the Committee's charge. The facilities considered were those that are national in scope, with initial costs on the order of $5-10 million or more, intended primarily for research on materials. However, materials research done on a laboratory scale is equally vital to the future strength of U.S. materials research. Support for laboratory-scale science is complementary to, not competitive with, the support for major facilities recommended in this report.

The relatively high costs of major facilities for materials research dictate that priorities be established; and the Committee in this report recommends priorities for major new facilities and new capabilities at existing facilities, for materials research and related fields. The recommended priorities involve three types of facilities, providing synchrotron radiation, neutrons, and high magnetic fields.

Synchrotron radiation, produced when energetic electrons are deflected by a magnetic field, provides over a broad spectral range the most intense source of photons now available. Such radiation can be intensified further by orders of magnitude by using insertion devices--wigglers and undulators--that put a series of sharp bends in the electron trajectories. Synchrotron-produced photons interact strongly with atomic electrons, thus, offering a means of probing the details of the electronic structure of materials.

In contrast, neutrons, which are produced by nuclear reactions, interact most strongly with atomic nucleii. Neutrons are thus uniquely

suited to the study of lattice dynamics and molecular configurations. In addition, since the neutron has a magnetic moment, neutron scattering offers a unique means of probing the magnetic properties of materials. The most effective use cold neutrons, which have very low velocities, requires that they be transported through special tubes, whose walls reflect those neutrons with minimum loss, to large experimental areas called guide halls.

High magnetic fields are essential to the study of a variety of technical and fundamental problems. In particular, high magnetic field facilities are essential to the development of improved superconductors and, in turn, make it possible to construct more efficient superconducting magnets capable of achieving still higher fields.

The Committee applied the following criteria in establishing its priorities:

- The importance of each facility for frontier research in materials, and consideration of research needs of other fields, including biology, chemistry, atomic and molecular physics, plasma physics, earth science, and medical science.

- The importance of each facility for applied research in areas of national priority; that is, economic competitiveness and security.

- The availability of other, less costly alternatives for accomplishing comparable scientific, technological, and educational goals.

- The contribution of each facility to a long-term national plan for such facilities, including considerations such as capital investment, operations costs, and technical feasibility.

Additional criteria that should be considered in evaluating proposals for new facilities include:

- Technical and scientific resources at the laboratory or university site, including schools or departments in related areas.

- Access and ease of use by extramural academic, industrial, or government laboratory investigators.

- Role of the facility relative to a new or strengthened mission of its home laboratory or university.

- Potential of each facility for training scientists and engineers.

Further, new facilities to be fully effective must be dedicated, that is, used exclusively for synchrotron radiation or neutron based

research. Finally, to serve the entire community optimally, the geographic distribution of facilities should generally be taken into account.

CONCLUSIONS AND RECOMMENDATIONS

The Committee's recommended priorities for major facilities--both new facilities and new capabilities at existing ones--embody two prerequisites:

- That they are accompanied by expanded support of smaller materials research programs, including related instrumentation. Research on this scale continues to provide much of the fundamental new science in the field and to train a large fraction of our scientific and technical manpower.

- That resources must be provided to operate existing user facilities productively. In addition, the approved enhancements of major synchrotron radiation facilities at the Brookhaven National Laboratory, Stanford University, and the University of Wisconsin should be completed expeditiously, since it will require several years to more than a decade before the new facilities recommended in this report can contribute to the research effort of the United States.

RECOMMENDED PRIORITIES

The Committee's recommended priorities for the development and construction of facilities during the next decade include two categories:

- Major new facilities, and

- New capabilities at existing facilities.

These categories complement one another in function, time scale, and required resources. New capabilities at existing facilities are essential for scientific and technological needs in the next decade, while the long lead times needed to construct major new synchrotron radiation and neutron facilities require that we start now with the planning and design of such new facilities. They also require that we begin immediately to implement new capabilities at existing facilities. The Committee concludes that both categories are essential for the effective evolution of science and advanced technology in the United States in the next decade and beyond.

The Committee also recommends the convening of additional panels to address other important aspects of materials research.

Major New Facilities

The Committee's recommendations for the construction of major new facilities are listed below in order of priority.

1. A 6 GeV Synchrotron Radiation Facility. This would be designed to make optimum use of the new scientific and technological opportunities presented by insertion devices. These devices, by providing radiation having orders of magnitude greater brightness than currently available, will make it possible to expand on the seminal research using synchrotron radiation carried out in the past decade. A synchrotron radiation facility with a storage ring energy of about 6 GeV will offer both identifiable and unforseeable new opportunities for research throughout the electromagnetic spectrum. It is optimal for providing radiation from undulators at about 10 keV, where most x-ray research is done. For example, the brightness increase will make it possible to investigate the properties of more complex materials and smaller samples with increased spatial and energy resolution. Site-independent design should begin immediately, and the site selection and construction should commence as soon as possible. If construction were to begin, for example, in FY 87, operation is possible by FY 92.

2. An Advanced Steady State Neutron Facility. The goal is to achieve about ten times the flux of existing machines with a minimum requirement of five times the flux. There are two principal reasons for this recommendation. First, and most important, a high-flux source can be designed to optimize beam geometry and flux distribution, so as to yield greatly increased intensities for all experiments. An increase of about ten times the flux of existing machines is an aggressive but technologically feasible goal. Such a facility would ensure the United States a leading position in this field. This is especially important in the cold neutron range, where flux increases of an order of magnitude can be achieved, providing new capability, for example, for high-resolution spectroscopy and small-angle scattering studies. Second, a new source will be a timely replacement for one or more of our existing sources built in the 1960's. Site-independent design should begin immediately. However, because of safety requirements, the Committee does not expect construction to begin until about FY 89 with completion possibly by FY 96.

3. A 1 to 2 GeV Synchrotron Radiation Facility. This facility would be centered around insertion devices but optimized for the vacuum ultraviolet (VUV) and soft x-ray region. This facility furnishes additional scientific and technical opportunities for research in chemical physics, electron spectroscopy, and imaging techniques such as microscopy and holography.

4. A High-Intensity Pulsed Neutron Facility. Pulsed neutron sources offer new scientific capabilities, especially for investigations requiring higher energy, or greater than thermal, neutrons. Also, there are practical limits to the intensity that steady state reactors can provide. Thus, future improvements in neutron sources, beyond the second priority above, will probably come from alternative approaches, the most promising of which is based on pulsed neutron

sources. However, future action on the construction of a high-intensity pulsed source (about 10^{17} neutrons/cm^2-sec peak flux) should be based upon the results obtained with lower-intensity pulsed sources.

New Capabilities at Existing Facilities

Recent developments make it both practical and cost effective to adapt certain existing user facilities to new purposes by adding experimental halls, instruments, and modified sources. These additions provide an opportunity for new frontier science; they are not simply extensions of existing work.

The Committee's recommendations in order of priority for the addition of these new capabilities at existing user facilities are:

1. Centers for Cold Neutron Research. Guide halls and instrumentation for exploiting the only cold neutron sources in the U.S. located at the Brookhaven National Laboratory and at the National Bureau of Standards, should be developed in an orderly fashion.

There is no cold neutron guide hall in the United States, and such facilities are urgently needed to address the rapid expansion of neutron applications in materials science, chemistry, and biology. Many central problems in these sciences can only be solved using new instruments with cold neutron beams. These centers will enable U.S. scientists to be competitive in cold neutron research during the next decade; and they will provide new instrumentation concepts for developing future neutron scattering sources.

2. Insertion Devices on Existing Synchrotron Radiation Facilities. Insertion devices should be developed in an orderly fashion to exploit about six of the remaining straight sections of existing storage rings. The special characteristics of undulators as radiation sources should be emphasized, to use our existing capability most effectively.

Undulators on existing machines will be our premier synchrotron radiation source for the next 5 years. They will also provide valuable experience for the next generation of synchrotron radiation facilities which will also be based upon undulators. The construction of additional insertion devices, when approved, should follow the construction of new capabilities at synchrotron radiation facilities already included in the budgets for FY 85 and FY 86.

3. Experimental Hall and Instrumentation at the Los Alamos National Laboratory. An experimental hall and new instruments at the pulsed neutron source at the Los Alamos National Laboratory (LANL) would make the United States competitive in pulsed neutron research and would help guide the development of future pulsed sources.

The expected flux increase at this facility is an important opportunity to explore, at modest cost, the great promise of pulsed neutron science for spectroscopic and structural problems.

4. Upgrading of the National Magnet Laboratory. The need for timely development of pulsed magnetic field facilities and instrumentation enhancements at the National Magnet Laboratory has been demonstrated. This laboratory, the only major high magnetic field research facility in the United States provides a unique combination of high fields and low temperatures. Many advances in research depend on its continued development as a dedicated user facility.

5. Enriched Pulsed Neutron Targets. Enriched targets, by exploiting fission events to amplify the neutron flux, can more than double the available flux. The development and installation of enriched targets for use at pulsed neutron facilities would be cost effective.

Priorities 1 and 2 for major new facilities, when they are implemented, would serve as a centerpiece of this nation's future capability for synchrotron radiation and neutron based research. Thus, design and siting studies for a 6 GeV synchrotron radiation facility and for an advanced steady state neutron facility should begin immediately.

Because of the long lead time associated with an advanced steady state neutron facility, the immediate implementation of at least one instrumented cold neutron guide hall is necessary to provide forefront capability.

The basis for these conclusions is expanded upon in the body of the report. Chapter I outlines the characteristics of materials research at universities, at governmental and private laboratories, and in industry, including research styles, research organizational modes, instrumentation, and the role of national facilities. It also offers a brief summary of the status of U.S. facilities vis-a-vis those of other countries. Chapter II outlines scientific and technological accomplishments, using major materials facilities, and suggests the likely direction of future research. It presents the scientific and technological rationale for the recommendations in this report. The Committee's conclusions and recommended priorities for national facilities for materials research and related fields are given in Chapter III.

The Committee again emphasizes that, in response to its charge, its recommended priorities include only synchrotron radiation, neutron scattering, and high magnetic field facilities. Other meritorious materials research facilities were also discussed by the Committee. A number of these are briefly described in Chapters I and III.

I. MATERIALS RESEARCH: FACILITIES AND MODES

Materials research is by its nature interdisciplinary, historically calling on expertise from engineering, physics, earth sciences, and chemistry and, recently, extending to biology and medicine.

In this chapter, we briefly describe the diverse research styles and types of facilities, instrumentation requirements, organizations, and modes of materials research. This is intended to set the context for the focus of the report: major neutron, synchrotron radiation, and high magnetic field facilities, costing in excess of about $5 million. These are all are national user facilities, each serving a group or groups of users whose interests often extend beyond the traditional materials research community. This focus responds to the charge to the committee, as stated in the opening sentences of the Preface and the Executive Summary.

Universities, the federal government, and private corporations are all involved in materials research. In universities, it is done in the main in different disciplinary departments. Within the government, it is done within facilities operated for the U.S. Department of Energy by private contractors, such as the Oak Ridge National Laboratory, the in-house laboratories of the Department of Defense, such as the Naval Research Laboratory, and other laboratories such as the National Bureau of Standards. Numerous industrial laboratories are also involved in materials research, usually in an interdisciplinary mode, ranging in focus from fundamental work to development and manufacturing.

UNIVERSITIES

Much of the materials research in the United States is done in small university laboratories, consisting of a few researchers and a total instrumentation inventory of less than $1 million. Research on this scale continues to provide important, fundamental new science and to train a large fraction of our scientific and technical manpower.

Universities have a crucial role in materials research. They are a major source of new ideas and concepts that often take years to mature, time that industry often cannot commit. And they are the sole source of future materials scientists and engineers. Universities also

operate special research facilities that are used by a broader research community.

Training new scientists and engineers for materials research is complicated by the needs of advanced technology for people who are broadly trained and fully conversant across the conventional disciplinary boundaries, such as, for example, condensed-matter physics and chemical engineering.

An important task for the universities is to develop stronger ties with industrial and governmental laboratories. Such cooperative programs stimulate new research, promote the exchange of new knowledge and technology, and help in thecontinuing education of mature technical personnel at industrial and governmental laboratories.

Materials Research Laboratories

The Materials Research Laboratory (MRL) program, supported by the National Science Foundation and the Department of Energy, is intended to stimulate interdisciplinary materials research within universities, of the sort not easily done under the traditional funding pattern of individual research projects. It emphasizes coherent, multi-investigator projects requiring collaboration among individuals in two or more materials-related disciplines. The MRL program has also emphasized the development of wellstaffed and well-equipped central research facilities, partly as mechanisms for stimulating collaboration. Finally, new projects can be quickly started with MRL funding including seed funds to assist both new faculty members and established faculty members with novel ideas or programs who wish to change research fields. MRL core support is not intended as a substitute for individual research project funding, but may properly catalyze significant new research initiatives. Several Materials Research Centers at universities are funded by the Department of Energy and by other agencies. A smaller kind of specialized program, the Materials Research Group, is currently under consideration by NSF.

Instrumentation for Materials Research*

The status of instrumentation in university research laboratories was examined in a 1971 study of the National Research Council (reference 23), commissioned by the National Science Foundation. At that time, a need for $200 million in new instrumentation was identified. Only a small fraction of the need was met at the time, leading to a more problematical situation now. Thus, in the intervening decade, the consumer

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* While this discussion of instrumentation focuses on the needs of the universities, many of the same problems are faced by governmental laboratories engaged in materials research.

price index rose by slightly more than a factor of three, while instrumentation costs inflated at almost twice that rate. The accumulated need is now at least $1 billion, and some estimates are considerably higher. The $1 billion estimate is what would be needed to bring university research laboratories up to modern standards and does not include the cost of major new facilities, such as reactors or accelerators. Results from a 1984 National Science Foundation instrumentation survey (reference 24) indicate that only 16 percent of current academic research equipment in the physical sciences could be characterized as "state of the art." Dealing with this crisis in university instrumentation is a matter of national urgency.

Small- and Large-Scale Instrumentation. Exacerbating the shortcomings in university instrumentation is the increasing need for new larger-scale instrumentation for small research groups, instrumentation that is expensive by traditional standards but modest by those of the national facilities. In some cases, the cost of such instrumentation, typically $250,000 to $1,000,000, will necessitate considerable sharing, usually with other investigators or groups at the same institution. Examples include electron microscopes, the new generations of high-powered or very fast lasers, equipment for studying specialized materials, such as molecular beam epitaxy or chemical vapor deposition apparatus, specialized environments such as "clean rooms," very high powered or pulsed magnets, and dedicated 32-bit superminicomputers.

The cost of equipping many experimental stations at large user laboratories is also in this category. For example, most of the beam lines at existing synchrotron radiation facilities now are financed by participating research teams from governmental, industry, and university laboratories. These groups provide their own funding for instrumenting ports to do particular kinds of experiments. It is expected that about half of the additional beam lines proposed in this report for the new and enhanced synchrotron radiation facilities will be funded by the research participants. Future neutron facilities may also be partly developed in this mode.

Large-Scale Computers. Over the past decade, a new and essentially different kind of instrument has been added to the increasingly complex instruments for experimental materials science: the large-scale computer, or supercomputer. Although simple properties of simple systems, such as the cohesive energies of elemental solids, can be calculated within about 10 hours with a 32-bit superminicomputer, calculations for more complex and interesting systems require vastly larger memory and increased computing speed. Greatly increased computing support, during the next 5 to 10 years, would qualitatively affect the usefulness of theory for the solution of materials problems.

Personnel

The need to fully use the facilities discussed here, coupled with the generally complex nature of modern materials research, implies a much more extensive use of technical and professional support staff in individual research groups than has been customary in the chemistry, physics, and materials science communities in universities. Biological scientists in universities are now well established in this mode of operation, as are many physical scientists in industrial and governmental laboratories.

FEDERAL LABORATORIES

The federally supported laboratories have widely diverse roles in U.S. materials science and technology, in keeping with the missions of their agencies. Thus, the national laboratories of the U.S. Department of Energy (DOE) conduct materials research related to the development of nuclear fission, fusion, and other energy sources, as well as to weapons. As do other federally supported laboratories, the DOE laboratories also operate special research facilities that are widely used by the broader scientific community. In fact, the special scientific or measurement capabilities, as well as the major facilities, of the federal laboratories, are the basis for their many cooperative research efforts with industry and universities.

The materials research and development activities of the laboratories of the Department of Defense (DOD) directly support general defense needs or particular weapon systems. Fundamental work in materials research centers on those activities areas inadequately addressed by the private sector or activities that may have an important long-range impact on the scientific or technological needs of future defense capabilities. Overall, the DOD laboratories can engage, when it is necessary, in all aspects of materials research and development, from fundamental concepts to providing prototypes. Finally, the direct role of the DOD in materials research is complemented by its indirect role in broadly supporting contract R&D at academic, industrial, and governmental laboratories of other agencies.

Other governmental departments and agencies also have major roles in materials research. For example, one of the central missions of the National Bureau of Standards, within the Department of Commerce, is research leading to new or improved measurement methods and standards and to basic understanding of the properties of materials needed by industry, universities, and government. The U.S. Geological Survey, within the Department of the Interior, has a major effort in basic and applied materials research related to the nation's mineral resources.

INDUSTRY

Condensed matter science is unusual in that a significant portion of basic research in the U.S. is performed in industry. This reflects the

fact that condensed matter science supports advanced technologies in many areas of national priority, including those of information systems, energy, health, transportation, and national security. Basic industrial research is conducted in all sub-areas of condensed matter science using many modes, ranging from the individual researcher to research groups. Industrial researchers also make active use of national facilities and collaborate in these efforts with university and governmental researchers. Multidisciplinary materials research is often carried out effectively at the major U.S. industrial research laboratories.

In addition to playing a major role in basic materials research, industry also helps define the future materials needed to advance important key technologies. That, in turn, serves as a guide to research at university and governmental laboratories as well as at industry laboratories.

The largest materials research effort in the U.S. undoubtedly is the industrial research and development effort focused upon product lines. Because this effort often requires advanced applications of materials for specialized uses, it generally requires a fundamental understanding of materials. The availability of university-trained scientific and technical personnel is essential for this extensive industrial research and development. Collaboration by industry researchers, with scientists and engineers at both university and governmental laboratories, contributes substantially to technology transfer. Recently, specialized facilities, such as microelectronics-related facilities, have been created at universities to address both basic research and the technology needs in industry.

MAJOR MATERIALS FACILITIES

Within the above perspectives on the diversity and range of facilities and practioners of materials research, the Committee describes below the status of several major materials facilities in the United States. These facilities are more fully described in a recent review article (reference 22).

Synchrotron Radiation Facilities

The synchrotron radiation facilities in the United States today range from small, virtually in-house facilities to large user facilities. The Cornell High Energy Synchrotron Source (CHESS) is a laboratory using a 5.5 GeV storage ring parasitically. The six end stations serve about 250 users annually. The National Synchrotron Light Source (NSLS) at the Brookhaven National Laboratory has two storage rings, 0.75 and 2.5 GeV, dedicated to the use of synchrotron radiation. Approximately 58 end stations, including those in a current upgrade program, serve a growing user community, currently estimated at 400 scientists annually. The Synchrotron Radiation Center (SRC) at the University of Wisconsin,

currently operates a 0.24 GeV storage ring and is commissioning a 0.75 to 1.0 GeV ring. The 20 beam lines on the latter serve an estimated 150 users annually. The Stanford Synchrotron Research Laboratory (SSRL), at the Stanford Linear Accelerator Center, uses a 3.5 GeV storage ring dedicated to synchrotron radiation part of the year and in a parasitic mode the rest of the year. Counting beam lines in a current upgrade program, the 19 end stations serve a user community of 300 scientists. In addition, one undulator beam line is to be built on a 15 GeV storage ring at the same site.

The Synchrotron Ultraviolet Radiation Facility (SURF), at the National Bureau of Standards, is a 0.24 GeV ring dedicated to synchrotron radiation use. Its 13 beam lines serve about 40 users annually. Expanded descriptions of these facilities and a definition and history of the user community, as well as its characteristics, can be found in two previous reports (references 5, 8).

Of the storage rings listed above, only three--two at NSLS and one at SRC--were designed to be sources of synchrotron radiation, and those three were all designed prior to a full recognition of the importance of insertion devices. Consequently, they were designed to emphasize the radiation from the bending magnets, with capabilities for the later addition of a limited number of insertion devices. (For a description of insertion devices, see Chapter II and references 5, 8, 18, 19, 20, 26.)

Foreign Synchrotron Radiation Facilities. Many synchrotron radiation facilities exist elsewhere, offering strong competition to U.S. scientists. These are extensively described in other reports (references 5, 8). The principal operating sources are in England (SRS), France (ACO, super ACO), West Germany (HASYLAB, BESSY), Japan (Photon Factory), and the USSR (VEPP-3, VEPP-4). There are other facilities in some of these countries, as well as in Italy and Sweden. Construction is under way for facilities in the People's Republic of China, and there are plans for facilities in Taiwan, India, and Brazil. None of the facilities mentioned above is more advanced than our newest facilities, NSLS and SRC. However, the European Science Foundation is planning to build a 5 to 6 GeV storage ring very similar to that proposed for the United States.

Neutron Scattering Facilities

There are, currently, active neutron scattering programs at five different national centers: Argonne (ANL), Brookhaven (BNL), Los Alamos (LANL), National Bureau of Standards (NBS), and Oak Ridge (ORNL). The BNL, NBS, and ORNL facilities center around steady state reactor sources, while ANL and LANL involve pulsed spallation sources. There are also reactor based neutron scattering programs at the University of Missouri, the Massachusetts Institute of Technology, and other universities. This section focuses on the national centers for neutron research.

The BNL facility centers around the 60 MW High Flux Beam Reactor (HFBR), which has a thermal flux of 1 X 10^{15} neutrons/cm^2-sec. It is equipped with eleven spectrometers and diffractometers, with two more under development. The NBS facility has nine end stations, with a tenth under development. A cold source has been installed on the BNL reactor, and funding has been provided for installation of a large volume cold source in the NBS reactor. The ORNL facility centers around the 100 MW High Flux Isotope Reactor (HFIR), which has a thermal flux of 1 X 10^{15} neutrons/cm^2-sec. It is equipped with nine scattering instruments, with a tenth under development. The instruments include a 30-meter small-angle scattering instrument that is funded by NSF as a national user facility. The ANL facility centers around a pulsed neutron source that produces bursts of neutrons with a peak thermal flux of 4 X 10^{14} neutrons/cm^2-sec at a 30 Hz repetition rate. It is now the most intense pulsed source in the world, equipped with eight instruments, with a cold moderator available for several beams. The LANL facility centers around a pulsed spallation source that, by 1986, will provide a peak thermal flux of about 1 X 10^{16} neutrons/cm^2-sec at 10 Hz. Six beam lines are now available, with two instruments operating in the user mode. Ten or more beam lines will ultimately be developed.

All of these centers have ancillary equipment, enabling one to study samples in varied environments with temperatures from 0.3K to 1800K, pressures up to 20 kbar, and magnetic fields up to 80 kG. There is extensive research by outside users at each center, with the individual center user programs varying from informal collaborations to a formal peer-reviewed process. In most cases, outside user experiments involve collaboration with in-house people.

Aside from the facilities described above, there are efforts at the various neutron centers to develop area detectors, multilayer polarizing monochromators, focusing collimators, and neutron choppers and polarizers, all of which are important for developing advanced instrumentation for reactor or pulsed sources. These efforts, in general, have a low-to-modest level of support and manpower compared with instrumentation projects in Europe, discussed below.

Foreign Neutron Scattering Facilities. This subsection offers a selective review of foreign neutron scattering facilities, concentrating on instrumentation developments particularly in Western Europe that have not been matched in the United States. An important key to the European success, especially at the Institut Laue Langevin (ILL), has been the development and use of cold neutron sources and associated guide halls to create instruments for ultra high-resolution and high-sensitivity spectroscopy. These currently provide energy resolutions as much as five orders of magnitude better than those available in the United States; they also enable studies of small-angle and medium-resolution diffraction and other new scientific applications. As already noted, there is only one cold neutron reactor source in the United States, at BNL, and another under development, at NBS.

The United States has no guide halls to improve the versatility and flexibility of cold or thermal neutron instruments. In contrast, 60 percent of the neutron scattering instruments at the ILL (reference 7) are located in a large guide hall, and a new guide hall and cold source are to be completed over the next 2 years. Also, there are major efforts at ILL to develop and construct focusing monochromators, polarizing devices, reflecting supermirrors, environmental control systems, dedicated instruments for diffraction surveys using neutron cameras, and more. Besides the ILL program, there is a new reactor center, called Orphee, at Saclay near Paris, with two hydrogen cold sources, which will ultimately commission over twenty new instruments for neutron scattering and fundamental physics research. Expanded guide halls with many new instruments are also under construction at the KFA Research Reactor in Julich and at the Berlin reactor. Finally, the Japanese government has approved funding for the complete modernization of the JAERI III Reactor at a cost of $150 million, including a replacement of the vessel, an upgraded fuel and beam tube arrangement, and installation of a large cold source and guide hall.

The total current operating expenditures for neutron scattering at research reactors in Western Europe is about $80 million per year, in FY 83 dollars, including associated reactor operation costs, roughly triple the U.S. effort. An order of magnitude difference emerges when one compares capital investment for new spectrometer development and construction efforts. The consequences of this investment gap over the past decade between European and U.S. research reactors are being felt increasingly in our inability to compete in many areas of new science involving such techniques as high-resolution neutron spectroscopy, small- and medium-angle diffraction, and diffuse scattering.

The current U.S. position in pulsed neutron research and development is better in relative terms with respect to foreign competitors than for steady state sources. For example, the Intense Pulsed Neutron Source (IPNS) at Argonne is presently the highest intensity facility in the world, and the Weapons Neutron Research/Proton Storage Ring (WNR/PSR) at Los Alamos is scheduled to provide, by 1987, an order of magnitude increase in intensity for pulsed neutron experiments.

However, developments abroad make current comparisons misleading. For example, the SNS advanced spallation source under construction at the Rutherford Laboratory in Britain, which is scheduled to be brought on line by the end of 1984, will have neutron intensities 2 to 3 times the current IPNS performance and will, by 1986, generate a peak thermal flux of 5×10^{15} neutrons/cm^2-sec at a 50 Hz repetition rate. That is roughly twice the total intensity of the scheduled WNR/PSR source. This facility will ultimately have a complement of at least 15 neutron scattering instruments. Moreover, the Japanese, who have developed a modest flux facility at Tsukuba with an impressive array of instruments, are also funding a planning and design study for a major new pulsed source, costing $100 million in FY 83 dollars, which would slightly exceed the characteristics of the SNS at the Rutherford Laboratory.

User Policy at Major Materials Facilities

Since major materials facilities are intended for a large community of scientists, it is very important that they be available to all qualified research investigators with meritorious proposals. A number of approaches have been used in the past to arrange participation, each having strengths and weaknesses. Some perspectives and generalizations from experiences to date are given below to help guide the formulation of future policies.

Criteria. There are several extant models of user policies for major neutron and synchrotron radiation facilities. In general, they satisfy the following generic criteria:

1. Experimental activities, except for construction and maintenance, whether they are initiated by research staff of the facility or by outside scientists, are presented and justified in written form. The proposals are reviewed before research is authorized and begun.
2. Committees reviewing proposals include a substantial fraction of scientists from outside the facility.
3. Priorities are established by the facility director based on ratings of the review committee and on scheduling considerations. The director has the discretion to provide for the insertion of experiments to exploit blocks of instrument time that are freed by unanticipated events.
4. Use of a facility is not restricted to U.S. scientists, but priority may be given to them in the event of equivalent proposals.
5. The time assigned for an experiment is designed to be adequate for the measurements, but extensive, repetitive, or confirmatory measurements may require the submission of additional proposals.
6. Some fraction of instrument time should be made available for use by the director at his or her discretion. This time can be used to extend assigned periods for current experiments, to permit preliminary experimentation in advance of a proposal, and for instrument development. Approximately 20 percent of instrument time is suggested for such purposes.
7. Users should be provided with an adequate level of technical support at the instrument so that they can safely and efficiently conduct experiments. Vacuum interlocks, shielding, and other safety devices should be controlled by facility management. The design of user facilities should make it impossible or difficult for any user at one port to affect the beam delivered to any other port.
8. The facility should provide a stock of standard test instruments, normal electronic and vacuum components, cryogenic fluids (liquid nitrogen and helium), data acquisition computer systems, commonly used gases, and some minimum storage space for user owned equipment.
9. It should be recognized that there are a range of user interactions. Some users will make very short-term and straightforward measurements, others will do long-term, interactive experiments in

which protocols and parameters are altered as the experiment proceeds. The different needs of these groups should be considered in designing facility user policy.

Participating Research Teams. A concept that has been used successfully in several major facilities is that of the participating research team, or PRT. This is a group of individuals who take communal responsibility for the design, construction, and operation of an instrument at an existing port. The PRT may also be responsible for organizing funding for the instrument. Industrial, university, and governmental groups have formed PRT's. It is a concept that appears to provide a reasonably successful approach to using facilities.

The principle is that, for a specified period--2 to 3 years, for example--the PRT has some 75 percent of the running time for that port, outsiders being allocated 25 percent. This has the advantage that the management of each instrument becomes much more flexible for members of the PRT, and more effective science may therefore be done. An important responsibility of the PRT's is to provide help for outside users. By augmenting the local staff in this manner, the entry barrier for naive users can be reduced. In some cases, PRT's are reviewed every 3 years for possible renewal; involvement with outside users is an important consideration in such renewals. A PRT is responsible for maintaining the instrument. If the PRT does not find its own outside users through collaborations, the facility director can assign an outsider to use the PRT's line during the open time.

Maximal use of a facility may involve a mixed mode operation in which some beam lines are operated by PRT's and some by the facility. The consequent flexibility of operation at the scientific level justifies the administrative complexity of such an arrangement.

Whatever the user policy, the experience to date indicates that it is important to keep the level of bureaucracy as low as possible, even if there is some loss of efficiency in using the instrumentation. This criterion tends to conflict with that of extensive peer review of lengthy proposals by potential users, so some balance is called for.

A mixed mode operation in which a facility has participating research teams and provides instruments seems an appropriate balance. It is not the intent of the Committee to spell out a rigid user policy for future major materials facilities. Any proposals for a new facility, however, should include a well-considered plan for utilization, taking into account the considerations mentioned above. The aim, of course, is to create user policies that permit the best science in an atmosphere of equal opportunity for different users.

II. MAJOR MATERIALS FACILITIES: SCIENCE AND TECHNOLOGY

Condensed-matter science, or materials research, deals with the diverse properties of solids and liquids and their interfaces. It is interdisciplinary, involving materials science, including metallurgy, ceramics, polymers; major subareas of physics and chemistry; as well as the earth sciences, biology, and medicine. Interest in materials research derives from fundamental science and technology. It is an intellectually stimulating area of science, as shown by the discoveries of fundamentally new phenomena, concepts, and states of matter during the past decade. Indeed, several recent Nobel prizes have been awarded for research in condensed-matter science.

Condensed-matter science supports advanced technologies in areas of national priority, including those of information systems, communication and computers, energy, health, transportation, and national security. Products of condensed-matter science, such as the transistor and the integrated circuit chip, have revolutionized our lives through their use in television, calculators, electronic watches, personal computers, appliances, autos, and innumerable other applications. In Table II.1, the Committee summarizes the connection between subareas of materials research using major facilities and technological applications.

SYNCHROTRON RADIATION, NEUTRON SCATTERING, AND MAGNETIC FIELDS

The spectroscopic analysis of matter involves bombardment with particles, such as neutrons or photons, with or without energy changes, or the use of high magnetic fields. The sensitivity that can be achieved is limited by the intensity of the radiation or the strength of the field.

Neutrons

The neutron is a unique probe that interacts weakly with atomic nuclei. The magnetic moment of the neutron makes it especially suited for examining magnetic properties of materials. By measuring changes in the

Table II.1. Connection Between Materials Research Subareas and Other Fields that Utilize Major Materials Facilities and Technological Applications of National Interest

	Information Systems (computers, communications, electronics)	Energy (fossil, nuclear, fusion, solar,...)	Health (Medical, Biotechnology, Environmental)	National Security	Transportation (ground, air, space)
Semiconductors	+	+	+	+	+
Metals and alloys	+	+	+	+	+
Insulators	+	+		+	+
Polymers	+	+	+	+	+
Ceramics	+	+		+	+
Magnetic Materials	+	+	+	+	+
Catalysts		+	+	+	+
Adsorbates		+	+	+	+
Lamellar (layered) materials	+	+		+	+
Composites		+	+	+	+
Biological molecules, macromolecules, and membranes			+		
Gaseous molecules and atoms	+	+	+	+	+
Plasmas (atoms, ions)		+	+	+	

* In addition to bulk materials, thin films, interfaces, and surfaces of several of the above materials are of major scientific and technological importance.

1208

momentum and energy of neutrons scattered by matter, direct information can be obtained on the structure of matter as well as its states of excitation.

For example, neutrons slowed to relatively low velocities--"cold neutrons"--have been used to "look" at the shapes of molten polymers. The technique is based on the fact that hydrogen and its heavier isotope, deuterium, scatter neutrons differently. Polymers are prepared in which hydrogen atoms are replaced by deuterium; isotope substitution does not alter the molecular configuration. Thus, when two polymers--ordinary and deuterated--are then exposed to a beam of cold neutrons, the actual size and configuration of the polymer can be deduced by comparing the different forms of neutron scattering from the two polymers.

Increased emphasis on research using cold neutrons is dependent on the availability of "guide halls," which are large experimental areas in which high resolution neutron spectrometers can be placed. This is possible because of the development of "guide tubes," which allow the neutrons to be transported many meters to the guide hall without significant loss of intensity.

Neutron beams can be either continuous or pulsed. Continuous beams are obtained from nuclear reactors, using controlled nuclear fission of uranium surrounded by suitable neutron moderators and reflectors, such as D_2 and beryllium. Pulsed neutron beams are generally produced from short bursts of high energy protons or electrons from an accelerator impinging on a heavy metal target, such as uranium or tungsten, to generate bursts of very high energy neutrons. This target is surrounded by a moderator-reflector assembly that is analogous to, but generally smaller than, that in a reactor, so that relatively short bursts of thermal and fast neutrons are produced at rates of 10 to 100 pulses per second.

Synchrotron Radiation

Synchrotron radiation is a unique source of photons, by virtue of its high intensity, brightness, stability, and broad energy range, extending from the far infrared to the x-ray region and beyond. It is created when charged particles within an electron accelerator are deflected by a magnetic field. The intensity of the synchrotron radiation can be further increased with the use of insertion devices. The simplest of these is the wiggler magnet that puts a relatively sharp kink in the electron trajectory of the synchrotron, thus increasing the radiation from that point. A more sophisticated device called an undulator in effect puts in a series of kinks so arranged that the light from each adds up in phase, giving an enormous increase in the intensity that can be achieved. Although synchrotron radiation represents a drain of energy in an accelerator, it was eventually recognized to be a source of intense radiation for new classes of experiments, first in solid state physics and then in other sciences.

Measurement of the moments and energy of synchrotron-produced photons, which interact strongly with electrons, provides information on structure and excitations. Such excitations range from molecular

vibrations, measured in the infrared, to the ejection of electrons from the innermost electron shells of atoms by photons in the x-ray region of the spectrum.

Such capabilities are very important for many fields. For example, synchrotron radiation is a major tool in probing the geometry and electronic structures of surface and solid-solid interfaces. In particular, photons from synchrotron radiation are used for photoelectron spectroscopy, in which electrons are ejected and their energy and angular distribution then measured.

Magnetic Fields

High magnetic field research is important for the fundamental understanding of a broad range of materials properties. Scientific advances in such diverse areas as superconductivity, permanent magnet research, and semiconductor science, all benefit from research based on the availability of intense magnetic fields. The attainment of such fields is ultimately connected to useful applications, development and industrial commercialization. Each time a higher magnetic field strength is achieved, it is quickly exploited by the scientific community and is accompanied by a requirement for yet higher field strengths. This new demand often requires a combination of high fields and low temperatures, or the combination of high magnetic fields with ancillary measuring equipment such as precision optical systems.

Superconductivity is the research area most strongly linked to high magnetic fields. An understanding of superconductors, which could form the basis for new and improved high field magnets, depends upon experiments carried out in some of the highest available fields. Therefore, the availability of present-day high field facilities is closely linked to the development of future facilities. High magnetic fields are also essential for probing those fundamental properties of superconductors that can be used to test microscopic theories, including theories based on the concept of electron pairing.

Basic Principles And New Problems

Against this background, it should be recognized that a family of basic principles and techniques underpins the field of materials research. Some of these have already been well exploited and are well understood. For example, the existence of lattice vibrations of short wavelength in metals was settled decisively with the use of neutrons some 25 years ago. Likewise, the electron energy band dispersions of solids and surfaces have been determined directly using photoelectron spectroscopy. Extended X-Ray Absorption Fine Structure (EXAFS) has been employed extensively to determine site-specific atomic structure for parts-per-million impurity concentrations and adsorbates. However, the applications of x-ray and neutron scattering to biology and polymer science, as well as to other aspects of materials science, are just beginning.

Effective, increased use of such techniques for improved understanding of fundamental biological processes will require the establishment of additional mechanisms for bridging between physical and biomedical scientists.

As theoretical concepts and processes for synthesizing materials advance, new problems come to the fore. Many involve the acquisition of detailed information regarding structural and dynamic properties that can be provided with the techniques employing neutron scattering, synchrotron radiation, or strong magnetic fields. Although it is impossible to forecast exactly how these techniques will be used to solve such problems, the Committee can predict confidently that there will be new problems a decade from now that will be especially amenable to approach with the equipment available at major materials facilities. The value of having equipment with advanced capabilities available to solve as yet barely discernible problems should not be underestimated. To indicate the breadth of applicability of such facilities, a partial list of available techniques is summarized in Table II.2.

Many problems that are well defined now cannot be explored adequately because the appropriate instrumentation or facilities are not available in the United States. Examples include the determination of the dynamics of intercalate species in single crystals of intercalated graphite having semiconducting properties. This problem can be approached using neutron scattering, along with nondestructive determinations of the concentration of electronic impurities in the range of 0.1 ppm using an x-ray microprobe.

In the following sections we discuss areas of science in which new major materials facilities can be expected to make further important contributions. More extensive summaries are described elsewhere (references 1, 2, 5, 7, 8, 18, 20).

SYNCHROTRON RADIATION RESEARCH: PAST AND FUTURE

Research with synchrotron radiation began in the 1960's and has grown dramatically in the past decade. Whenever a synchrotron radiation facility offering an increase in brightness, typically by a factor of from 10 to 10,000, became available, new types of research became possible. Furthermore, experiments carried out with such new equipment have usually demonstrated how new science could be developed if still higher brightness was available.

Four Generations

We have gone through three generations of such increases in brightness; the fourth is at hand. The first was associated with synchrotron radiation from the bending magnets of storage rings built for particle or nuclear physics. The second came with the construction of new storage rings specifically intended to produce synchrotron radiation (reference 1). These are now in operation or soon will be. The third emerged with the realization that insertion devices, wigglers and undulators

TABLE II.2. Techniques Available at Synchrotron Radiation and Neutron Facilities

		Neutrons	Photons: X-ray	Photons: Soft X-ray and VUV
I.	Elastic scattering*			
	Bulk crystallography	x	x	
	Surface crystallography	x	x	
	Molecular cystallography	x	x	
	Small angle scattering	x	x	
	Polarized scattering	x		
	Magnetic scattering	x		
	Diffuse scattering	x	x	
II.	Quasielastic scattering			
	Diffusion	x		
	Reorientation	x		
	Critical dynamics	x		
III.	Spectroscopy and elemental analysis			
	Inelastic (E,k) scattering			
	- electrons		x	x
	- phonons	x		
	- magnons	x		
	Absorption, reflection, fluorescence		x	x
	Absorption spectroscopy			
	- EXAFS		x	x
	- SEXAFS		x	x
	- PHD		x	x
	Photoelectron spectroscopy			
	- core level		x	x
	- valence level		x	x
	- ARPES		x	x
	- yield spectroscopy		x	x
	Photon stimulated desorption			x
	Photo chemistry		x	x
	Activation analysis			
	- thermal neutron activation	x		
	- prompt γ-ray	x		
	- fast neutron activation	x		
	- nuclear track	x		
IV.	Imaging and microscopy			
	Microscopy			x
	Microprobe		x	x
	Depth profiling	x	x	
	Topography	x	x	

TABLE II.2 (continued)

		Neutrons	Photons: X-ray	Photons: Soft X-ray and VUV
IV.	Imaging and microscopy (continued)			
	Lithography			x
	Interferometry	x	x	
	Radiography	x	x	
	Autoradiography	x		
	Holography			x
V.	Radiation effects			
	Radiation damage	x	x	x
	Isotope production	x		
	Transmutation doping	x		

* Many of the elastic and inelastic scattering techniques can be time resolved and/or spatially resolved with increased resolution and usefulness as the brightnesses of future sources are increased.

(see references 5, 8, 17, 18, 19), would enhance the intensity of synchrotron radiation. These devices have been, and are being, added to the present generation of storage rings, although not yet to the maximum possible degree. Unfortunately, the appreciation of the role insertion devices could play came too late to influence in any major way the design and construction of our present generation of storage rings.

The fourth generation of synchrotron radiation facilities, now technologically possible, involves the construction of new storage rings designed to maximize the brightness of the radiation from insertion devices. Such rings offer brightness increases by factors of from 50 to more than 100 over the best synchrotron radiation sources we have today or that we can achieve by adding new insertion devices to existing facilities. No dedicated facility that can produce undulator quality radiation in the x-ray region exists at present. Using the orders of magnitude increase in brightness that will be achieved with a new 6 GeV facility, we will be able to conduct entirely new types of experiments, some of which will open up major new research areas.

Synchrotron radiation has already contributed to many aspects of materials science as well as to other fields. Some of the more important contributions are outlined below. More extensive descriptions may be found in references 5, 8, 18, and 20, and in the references therein.

The simplest experiment, and one of great importance, centers about the measurement of photoabsorption by atoms, molecules, and solids. The continuum of synchrotron radiation allows easy access to the core levels of many atoms and has revealed a variety of many-body phenomena, including giant collective resonances, so-called Fano (interference) line shapes, "missing" spectral lines, and the "spike" shape of some absorption edges in metals. These have contributed to a better understanding of many-body effects in both atoms and solids.

At energies above the absorption edges in solids, the extended x-ray absorption fine structure (EXAFS), which is produced by interference effects in the scattering of the ejected core electron, gives precise information concerning the local geometry of the absorbing atom. When increased brightness is available, the EXAFS technique can be extended to detect elements in bulk samples and submonolayer adsorbates on surfaces that are present in concentrations of parts per million. EXAFS gives site-specific, geometrical information regarding atoms in samples of many types, such as coal, alloys, catalysts, and biological molecules. In most cases, the structural information obtained with the EXAFS technique was unattainable previously. Examples include geometrical information concerning the active site of the important nitrogen-fixing enzyme, nitrogenase; information relative to the active sites of important catalysts; structural parameters of impurities in coal and oil that make processing difficult; and studies of the role of impurities in determining important mechanical properties of materials.

Photoemission spectroscopy is widely employed at synchrotron radiation facilities. It provides independent information on initial and final electron states. Moreover, the anisotropy exhibited by

atomic and molecular photoemission spectra gives information concerning atomic wave functions that is different from that obtained from absorption spectra.

Photoemission from molecules exhibits shape-dependent resonances that are studied in the gas phase and then used to determine the orientation of molecules on surfaces. The continuum of synchrotron radiation makes possible various forms of so called "yield spectroscopy," in which the absorption of photons is signalled by secondary events. In this way, one can, for example, selectively examine absorption in the region of a surface by monitoring the yield of Auger electrons. Similarly, one can determine the onset of bulk absorption by monitoring the emission of characteristic x-rays. Brighter synchrotron radiation sources have permitted angle-resolved photoemission experiments that give electronic band structure, including symmetry, directly from the data. These experiments yield fundamental energy band information for solids, surfaces, and adsorbates, and thereby provide the basis for a more complete understanding the electronic properties of matter.

While EXAFS and photoemission spectroscopies have been pursued since the advent of x-ray and VUV synchrotron radiation based research, x-ray scattering and direct imaging technologies are just beginning to be carried out with the newest generation of insertion devices and storage rings. In spite of the limited time in which they have been available for exploration, these facilities have already shown that they can be used to obtain significant results. This gives us confidence that research based on synchrotron radiation will benefit dramatically from the next generation of facilities employing insertion devices. The scattering of x-rays by monolayer adsorbates and freely suspended thin films that are two monolayers thick has already been successfully demonstrated. In addition to opening the techniques of x-ray crystallography to the world of surfaces, thin films, and interfaces, synchrotron radiation has permitted exploration of the scientifically important phenomena associated with two-dimensional phase transitions.

The increase in intensity offered by the newest storage rings has enabled the study of bulk crystals that are as small as 1 μm^3 in size, thus permitting the determination of the structure of many important materials, such as zeolites, that can only be grown in the form of very small crystals at present. The use of anomalous x-ray scattering promises to help solve the difficult problem of determining scattering phases that has plagued crystallographic studies of important large macromolecular systems. The pulsed nature of synchrotron radiation has been used successfully to study the technologically important process of laser annealing of silicon as well as the scientifically important problem of muscle action in animals. The initial experiments in which synchrotron radiation is used for angiography have shown real promise of improving this medically important diagnostic procedure dramatically (reference 8).

Summing up, the first three generations of synchrotron radiation have already provided us with a revolution in the capabilities for using photoemission and EXAFS techniques and have demonstrated great promise for employing scattering and imaging to advance many areas of

science and technology. Insertion devices, particularly undulators, will advance the areas approachable with the use of photoemission and EXAFS techniques further and provide dramatic new opportunities for scattering and imaging.

The topics described above indicate what can be done with the newest sources of synchrotron radiation. More important are the even more complex research problems that can be undertaken with new storage rings that are designed specifically to use insertion devices. Examples are given below.

Condensed-Matter Physics

A major fraction of research using synchrotron radiation, both x-ray and soft x-ray, has involved the field of condensed-matter physics. There is a large number of new applications that cannot be addressed because of limitations of sources or instrumentation, or both.

Photoemission Spectroscopy. Photoemission spectroscopy is the primary technique for studying the electronic structure of solids, surfaces, adsorbates, and interfaces. On the basis of experiments being carried out at the new synchrotron radiation facilities, we can foresee what can be done with yet brighter sources. Angle-resolved photoemission provides understanding of the electronic band structure, including the band structure of the surface. The sample may be a crystal or an ordered overlayer. The resolution of angular and energy distributions has been increased with sources of higher brightness and have revealed new structures. Additional resolution is mandatory for the study of any material with a large unit cell, either in the interior or on reconstructed surfaces. Recently, measurements of spin-polarized photoemission have been carried out with synchrotron radiation. When combined with angle resolution, this procedure allows determination of the band structure of magnetic materials, including the spin labels for the bands. This is a technically difficult experiment. In particular, polarization detectors are notoriously inefficient. Brighter sources are mandatory if this technique is to be used widely.

At higher photon energies, one enters the region of x-ray photoemission in which the binding energies of core levels and the density of states for the valence electrons may be probed. Commercial equipment for this type of measurement with a resolution of approximately 0.5 eV at fixed photon energies is available. A synchrotron radiation source of the next generation would offer both higher resolution and higher sensitivity than anything possible today, thereby improving the utility of this already useful spectroscopy. Of perhaps greater significance is the extension of photoemission spectroscopy to procedures providing time and space resolution. This would make it possible to study surface reactions and to carry out microprobe studies of photoemission.

Surface Science. Other techniques for the study of surfaces also are benefitting from higher brightness sources. One is surface EXAFS, in which an absorbed x-ray excites a surface atom or molecule and a fluorescent x-ray or an Auger electron is then detected. The spectra give precise geometrical information on the location of the surface species. Photoelectron diffraction gives similar information. Both these techniques provide gains in surface sensitivity as the source brightness increases, and allow the study of surface species at ever great dilution. Finally, the new areas of photon-stimulated desorption of species from the surface requires sources of higher brightness. Both neutral and charged atoms and molecules, in their ground and excited states, can desorb from surfaces during photoabsorption. This may be the most site-specific surface phenomenon known. The photon flux used must be high because of the possibly small number of desorption sites and the low probability of release.

X-ray Scattering. X-ray sources of higher brightness are ushering in a new era in x-ray scattering. One can now work with surfaces, thin overlayers, and even freely suspended membranes. The crystallography of reconstructed surfaces can be determined, as can that of monolayer adsorbates. Thus, the crystallographic technique responsible for determining most of the known bulk structures can be extended to surfaces and thin films with insertion devices. This can be done as a function of temperature, to follow the structure and dynamics of quasi-two-dimensional melting. In fact, the study of phase transitions in two dimensions is providing important tests of theories of the behavior of the two-dimensional world of surfaces and thin films. Magnetic x-ray diffraction has been observed recently on the 54 pole wiggler at Stanford and promises to be comparatively routine when the brightest available x-ray wiggler sources can be used. Magnetic diffraction can provide much information concerning the magnetic structures of solids when an x-ray undulator on a 6 GeV source is available, and thus will complement traditional neutron studies, especially for materials for which only small samples are available. In some cases, surface magnetism may also be studied.

Inelastic X-ray Scattering. One field almost completely neglected in the first three phases of the evolution of synchrotron radiation has been inelastic x-ray scattering as related to the dynamic properties of the system being studied. The brightness of the radiation is most important for such research. Inelastic scattering of x-rays can, in principle, be used to probe both the electronic properties, such as those of plasmons, as well as collective atomic properties, such as lattice vibrations. However, achieving the 10^{-2} to 10^{-3} eV energy resolution needed will require the brightness provided by insertion devices and by major new instrumentation.

Atomic and Molecular Physics and Chemistry

Gas-phase photoemission has contributed extensively to our knowledge of atoms and molecules. Early studies emphasized the "static" study of excited states, the decay channels being inferred from line shapes. As the brightness of sources increased, the decay products, such as ions, electrons, and photons, could be detected. Finally, coincidence experiments began to be carried out, leading to more precise information regarding the nature of the excited states. Gas-phase experiments always require high brightness sources, for the sample is necessarily dilute.

The next-generation sources will permit several new classes of experiments. We already can work with gases at high enough resolution to excite single vibronic levels in molecules. These excited states can then be probed by high-resolution laser-spectroscopic techniques. Moreover, when source brightness becomes adequate, a molecule in an excited state can be made to interact with another molecule, bringing in an era of state-to-state photochemistry. These experiments are not possible with present sources because none have adequate brightness. Moreover, the time structure is not favorable.

The next-generation source will have pulse lengths shorter by a factor of about five relative to those now available. Such time structure will permit fluorescence spectroscopy from excited states on a time scale of a few picoseconds--shorter than the radiation pulse itself. This capability will, for example, make it possible to determine structural and dynamic properties of large molecules in solution and to study atomic and molecular reactions on surfaces. It will also be possible to use molecular beam techniques.

Biology and Medicine

EXAFS and x-ray crystallography involving synchrotron radiation have been applied to biological systems in the past. EXAFS has been useful for obtaining detailed information on large biomolecules such as hemoglobin. It is especially useful for molecules with a functionally important minority constituent, such as a metal atom in an enzyme. With increasing source brightness, it is possible to work with larger molecules having fewer active elements per unit volume. Time-dependent studies in which the structural response of the active site in the molecule to a chemical perturbation is determined become possible. Time-dependent x-ray absorption spectroscopy has already been used to follow the Fe absorption edge as the iron in myoglobin recombines with CO after laser-induced flash photolysis of carboxymyoglobin (references 25, 26). This was done on a 300 sec time scale with an existing storage ring. Better time resolution is possible, but EXAFS measurements on such a time scale await a source with higher brightness.

In studying x-ray damage to biological molecules and crystals, it has been found recently that the reciprocity law breaks down, and less damage results if the radiation dose is delivered at high rates for a

short time. Therefore, higher-brightness sources offer the opportunity to work with smaller crystals, including those of molecules difficult to crystallize. They also make it possible to collect more data before samples become so badly damaged as to impair resolution.

Element-specific imaging represents the principal foreseeable application of synchrotron radiation to medicine. One form of coronary angiography used today involves the imaging of the coronary arteries in real time by K-edge absorption of iodine which is added to the blood. The classical technique is invasive, and provides relatively low resolution. In-vivo angiographic studies of animal hearts with synchrotron radiation are noninvasive, fast, and provide higher resolution. Studies on human hearts are planned and, if they are successful, should provide novel approaches to studies of atherosclerosis and, eventually, to clinical applications. A high-field wiggler would represent the only foreseeable source for such work with present machines, but bending-magnet radiation from a 6 GeV ring could facilitate applications of this technique.

Earth Sciences

The earth sciences provide opportunities for the application of synchrotron radiation in connection with microprobe analysis. Such analysis is now carried out with electron microprobes. Synchrotron radiation can also be used in x-ray diffraction studies at high pressures. Higher brightness than is now available will benefit such research.

Imaging and X-ray Microscopy

There are several methods for achieving element-specific imaging, all at a relatively primitive stage of development. These include microprobe analysis, microscopy with zone-plates, and contact "lithography." As source brightness grows and the coherence of the radiation from soft x-ray undulators increases, microscopic holography and soft x-ray diffraction will become feasible. Both processes promise to give three-dimensional images of microscopic biological elements with a spatial resolution down to about 50 Angstroms. Available new sources will allow demonstrations of these techniques, which can be applied to study phenomena within a single cell. An undulator on a next-generation storage ring will make it possible to carry out useful and wide-ranging studies on such systems, employing radiation that "sees" only one element at a time.

Electron microscopy cannot be applied readily to living cells. However, holographic imaging techniques may make it possible to work with living cells, or at least with cells that have been processed less than is now the norm in electron microscopy. The imaging can be carried out on a millisecond time scale and with submicron resolution. The source needed for such imaging, an undulator on a 1 to 2 GeV next-generation storage ring, will have coherence properties similar to

those believed achievable with VUV and soft x-ray harmonics of visible and UV lasers. In fact, at shorter wavelengths, the undulator should provide higher average power than laser based sources (reference 27).

The foregoing selective examples show that synchrotron radiation is used for many purposes by scientists from a variety of disciplines. Research groups are combining the use of synchrotron radiation with other techniques, such as molecular beam epitaxy, pulsed lasers, and electron energy loss spectroscopy.

The versatility and power of research based on the characteristics of synchrotron radiation have emerged in the past 15 years. With the new capability provided by insertion devices, primarily undulators, the future impact of these devices will be even more profound.

NEUTRON SCATTERING RESEARCH: PAST AND FUTURE

Worldwide neutron scattering facilities and research applications have grown dramatically during the past decade. The most notable example is the emergence of the British/French/German center at the Institut Laue Langevin at Grenoble. But the Grenoble facility is only part of a major transformation of the field throughout Western Europe and more recently in the United States and Japan.

A New Generation Of Instruments: Europe And The United States

Over the past 25 years, the unique characteristics of the neutron as a probe of condensed matter has transformed much of our fundamental understanding of the physics and chemistry of materials. In keeping with this, a new generation of cold and thermal neutron instruments has been developed during the last decade, particularly in Europe. These have extended the wavevector range and energy resolution for neutron experiments by orders of magnitude. And they have, in turn, made possible new research in physics and chemistry and greatly expanded the applications of neutron scattering to new areas--materials science, polymers, and biology. Thus, the neutron scattering community in Europe has tripled in the past decade, and, more recently, the neutron scattering community in the United States has nearly doubled. This growth has also been stimulated by the emergence of higher-intensity pulsed neutron sources which by providing higher neutron energies have created new opportunities for neutron scattering research (reference 7).

The emphasis at current steady state reactor centers in the United States has been primarily on forefront research rather than on the development of instrumentation. This has been dictated, in part, by the U.S. neutron funding profile. By necessity, and in contrast, the pulsed source programs at Argonne and Los Alamos have emphasized development of pulsed source instrumentation and techniques, although important research has also been accomplished there.

Early neutron scattering research focused primarily on the exploration of basic issues in condensed-matter science. These issues

included phonon and magnon dispersion relations, the structure of hydrogenous materials, crystallographic and magnetic structures in simple solids, and phase transitions in model systems. In the past decade, the range of systems under examination has broadened considerably, and the scientific issues have often become much subtler. Neutron scattering has thus become an essential tool, providing unique structural and dynamical information central to the elucidation of the physics, chemistry, and other attributes of systems that are typically of interest to very broad communities. This change in character is evident in the outstanding accomplishments involving the use of neutrons in the last decade at major centers around the world.

These accomplishments include elucidation of (a) the structures and transitions in magnetic superconductors, (b) the physics of disordered magnets including metallic glasses, percolating alloys, spin glasses, and random field magnets, (c) the structures and excitations of incommensurate systems, especially those involving one-dimensional mass and charge density waves, (d) tunneling modes in chemical systems, including deuterated solid methane and hydrogen trapped by impurities in metals, (e) stoichiometric rearrangement and diffusion mechanisms in fast ion conductors, (f) early stage nucleation of voids in metals, (g) single polymer chain configurations in bulk polymers as well as composite polymer materials, (h) the spatial organization of macromolecular assemblies such as ribosomes, and (i) the location and exchange of hydrogen in proteins.

Finally, there have been important contributions to basic particle physics, including the determination of an upper limit on the electric dipole moment of the neutron, an upper limit on the occurrence of nonlinear terms in the Schrödinger equation and limitations on the incorporation of gravity in the Schrödinger equation. In all of these cases, neutrons have played an essential role.

In spite of major contributions to these and other impressive accomplishments, the current state of the U.S. neutron facilities is unsatisfactory. The broadening of the scientific base of neutron scattering necessitates the development of new capabilities at existing facilities with a new generation of instrumentation. Further, by the mid-1990's our existing reactor sources will be 25 to 30 years old, so that their long-term viability becomes a serious issue. In addition, many experiments of current interest turn out to be signal- or resolution-limited, so that greatly increased fluxes are required. This can be achieved by developing a new steady state reactor and a new pulsed spallation source.

Against the above summary of past accomplishments, the Committee describes areas of materials research and other fields in which neutrons can be expected to make important future contributions if advanced instrumentation and new facilities are developed in the United States.

Condensed-Matter Physics

A major fraction of neutron scattering research traditionally has been directed toward condensed-matter physics. Concomitantly, there is a continuous stream of interesting and important physics problems for which neutrons provide essential information. There are, however, a quite large number of problems in condensed-matter physics of immediate importance that cannot currently be addressed in the United States because of limitations on instrumentation or flux. This class of problems is discussed below with emphasis on four research areas.

First, as a result of rapid progress in the techniques of materials fabrication, a remarkable variety of lamellar materials can be synthesized. In all of these, there are important structural and lattice dynamical questions that often can be addressed only with the use of neutron scattering. Examples include artificial multilayer materials such as GaAs/GaAl$_x$As$_{1-x}$, and CuNi. High-resolution studies of superlattice effects in the phonon dispersion relations are surely needed. Other important low-dimensional systems include graphite intercalation compounds of which very high quality but rather small (about 0.5 mm^3) single crystals have recently been produced, and also hexatic smectic liquid crystals. Studies of in-plane dynamics of the intercalates and of excitations in hexatic phases would yield fundamentally new results. A related and rapidly-growing area of research centers about the determination of the structure and dynamics of adsorbed species of molecules, especially hydrocarbons on high surface area substrates. All such studies would require high resolution and a copious flux of cold neutrons.

Second, in studying highly disordered magnets involving competing interactions, such as spin glasses and random field magnets, it has been found that important new effects occur in the time domain; for example, the system gradually freezes into a metastable state with decreasing temperature. Moreover, pronounced hysteresis effects that depend on the prior history of the sample are observed. This class of problems, which promises to grow in importance over the next decade, requires use of the very high energy resolution provided by the spin-echo technique.

A third new area of materials research relates to the study of nonequilibrium phenomena such as spinodal decomposition in supersatured alloys and turbulent flow in anisotropic liquids. The advent of wide angle position-sensitive detectors and modern data acquisition systems provides important new opportunities for such studies. Using a next-generation reactor source, one may expect to collect complete powder diffraction or small-angle scattering patterns with reasonable statistical accuracy for periods of time between 0.01 and 0.1 sec. This will allow probing the early time behavior of such systems.

A fourth area of research that has always been severely limited by both flux and instrumentation is the scattering of polarized neutrons. Polarized neutron techniques allow separating magnetic and nuclear scattering as well as coherent scattering and incoherent scattering arising from nuclear spins. An order of magnitude increase in flux, with improved polarizers for neutrons of short wavelength, would

make many new experiments possible. Examples include studies of the excitations in magnets above the thermal transition temperature, elucidation of the spin dynamics in rare earth materials with mixed valences, separation of the magnetic scattering in spin glasses, and studies of magnetic defects in antiferromagnets.

There are, of course, always many important materials where, in spite of the best efforts of crystal growers, small sample size limits or prevents the full range of useful neutron experiments. Examples include Nb_3Sn, Nb_3Sb, $MEM(TCNQ)_2$, $ErRh_4B_4$, as well as others mentioned above. An order of magnitude increase in flux would bring many such problems into reach.

Finally, the increased neutron flux in the epithermal range will enable access to important new information on high-energy magnetic excitations in transition metals, actinide compounds, rare earth metals, and intermetallic compounds. Experiments involving the determination of the single particle momentum distribution in He^4 and He^3 as well as other light atom systems can also be anticipated.

Materials Science

Polymer and Colloid Science. The availability of small-angle neutron scattering (SANS) facilities has led to revolutionary advances in polymer science over the past decade. As indicated earlier, the substitution of deuterium for hydrogen makes it possible to extract information concerning the global molecular geometry of polymer molecules in the presence of high concentrations of other polymer molecules having the same chemical structure but differing isotopic compositions. There are at present no other experimental methods for making such measurements. Results have stimulated significant advances in understanding that, in turn, have led to new experiments. These SANS experiments have been carried out primarily on an instrumented cold neutron guide at Grenoble, although useful work has been achieved at new U.S. facilities. Important accomplishments include measurements of the conformation of single molecules in dilute and concentrated solutions and in amorphous bulk polymers. The state of miscibility of polymer blends and the state of aggregation of polymeric superstructures can also be characterized.

Extensive exploration of molecular interactions and phase diagrams over a range of temperature, concentration, and pressure will be required in the future. Those experiments will be dependent on greatly increased fluxes to achieve realistic data collection times. There is also a compelling need for studies of the dynamics of polymeric systems in real time--including phase transformation rates, deformation rates, annealing, and conformational changes. Measurements at lower wave vectors (q) are also needed to enable one to look at progressively larger polymeric molecules. Such new applications require modern SANS instruments located on cold source guide tubes with copious fluxes.

So far, only a limited number of low-energy inelastic scattering experiments have been reported in polymers. Here one is especially interested in low frequency motion in which long sections of the polymer

molecule move in concert. Real advances require the development of spin-echo spectrometers, which also incorporate high-q resolution, along with back-reflection spectrometry having high-energy resolution. Quasi-elastic neutron scattering instruments covering an extended q range, from 0.01 to 2 Angstroms^{-1}, could, for example, provide an integrated understanding of the high-frequency motions that determine the chemical and electrical properties of polymers, and the low-frequency motions that dominate their mechanical and transport properties.

Metals, Alloys, Ceramics. The start-up of the high-flux, SANS instrument at Grenoble in the 1970's, along with earlier ground-breaking work at Jülich and Saclay, marked a turning point in the use of neutrons for studying structural and related problems in metals and alloys. These instruments made it possible to examine heterogeneities in bulk samples at small wave-vectors without multiple scattering. Important failure mechanisms in these materials are associated with the formation of small voids, often located at grain boundaries. These include radiation damage, hydrogen charging effects, high temperature fatigue, and creep. In the past, the small size of these pores and their low fractional volume made it difficult, if not impossible to obtain statistical information or to follow the growth and linkage leading to failure. Such studies are vital to test competing theories in these areas.

Another important use of SANS has occurred in the study of clustering and precipitation phenomena in alloys as well as in the investigation of internal oxidation. Here, again, important tests of theory, such as scaling laws, are occurring. Activities by U.S. scientists in this growing field which uses SANS facilities recently developed in this country, as well as the Grenoble instrument in Europe when available, to obtain additional sensitivity or resolution, are already making major contributions.

In spite of the progress that has already been made, the application of SANS to the study of microstructure and distributed damage in real engineering materials is at an early stage. There is a need to investigate the formation of voids and precipitates in steel and other structural alloys from a very early stage of development, emphasizing size and volume fraction. The exploitation of this and other major opportunities in the next decade will require the development in the United States of much higher intensities of neutrons of long wavelength, along with more efficient and effective collimation and area detection systems.

The attainment of much higher intensity SANS instruments will also permit the kinetics of processes such as precipitation, phase decomposition, and grain coarsening to be followed in real time, on a scale of about 0.1 sec or greater, under realistic conditions of temperature and stress. Higher sensitivity and resolution, as well as longer neutron wavelengths, will be needed to test models of damage accumulation that lead to failure of materials and of structures. Such capabilities will also be important for new areas, making possible, for

example, in-situ studies of densification of ceramics at various stages of processing.

Other recent advances include the rapid development of high-resolution powder diffraction equipment at pulsed neutron and reactor sources. This not only permits the determination of the structure of materials such as complex ceramics and catalysts, which cannot be obtained in single crystal form, but also makes possible the study of residual and interaction stresses as a function of depth in metals and multiphase materials. Energy-dispersive pulsed source techniques have proven to be particularly useful in many of these studies. It is clear that such investigations will increase in importance in the next decade, particularly as much higher neutron intensities become available, allowing the stresses in smaller-volume elements in structural materials, and more complex structures, to be probed.

Chemistry

The most exciting opportunities for applying neutron scattering to condensed-matter chemistry in the next decade will require the development of instrumentation with very high resolution and high sensitivity for both elastic and inelastic scattering. In dynamic studies, this is particularly true for low energy cold neutron spectroscopy (0 to 20 meV) and quasi-elastic scattering, in which the use of neutrons provides unique information relative to other approaches. There is a growing interest in fundamental studies of rotational processes and interactions, tunneling phenomena, and ionic and molecular diffusion mechanisms in solids, as well as of molecular species bound in homogeneous and heterogeneous chemical media. The study of the dynamics of such systems on an atomic and molecular scale is of great importance, for example, in gaining understanding of the behavior and activity of catalysts and chemical absorbents, as well as of intercalated and layered materials. The studies will require energy resolutions between 0.1 μV and 0.1 meV, depending on the dynamic modes or processes being investigated.

Future applications of high-energy neutrons to determine vibrational spectra using pulsed or reactor sources will require considerably higher resolution as well as spectral measurements for variable wave-vector transfers. Experiments carried out under these conditions require much higher neutron fluxes to allow accurate measurements of line shapes and spectral intensities. This will, in turn, be necessary to test dynamic models of molecules bound in chemical systems. Moreover, many of the future applications of neutron scattering in chemistry will involve the measurement of high-resolution difference spectra, in which the signal from the species of interest is small in comparison with that from the surrounding medium. This small signal, coupled with the often small sample sizes, will accentuate the need for higher neutron intensities and new instruments. Measurement of difference spectra will make it possible, for example, to study the bonding, diffusion, and interaction of molecular species adsorbed in supported catalysts, as a function of the size of the catalyzing metal

particles. Systematic studies using different catalysts, supporting substrates, and impurities are also of great interest.

In chemical crystallography, one of the requirements for neutron research in the next decade will be the extension of powder diffraction studies to ever higher resolution, so that more complex structures can be determined under wide ranges of temperature and pressure, for example, in ionic conductors, ceramics, catalysts, and even organic solids. High-resolution instruments will also be required to evaluate the details of disorder in complex stoichiometric and nonstoichiometric materials. For example, such new instruments will aid in the determination of the effect of incommensurate arrangements of oxygen and metal atoms in ceramics on the chemistry of these materials, such as titanates and niobates. In addition, studies of small single crystals, less than about 1 mm^3, of many new materials, including ceramics and inorganic complexes, will be required. Finally, there is a growing interest in real time, in-situ studies of atomic rearrangements occurring during solid state chemical reactions. All of these emerging applications require higher-intensity beams and greatly extended use of high-efficiency detectors and multidetector analyzers.

In the area of molecular liquids, the investigation of the relationships in dynamical behaviors of complex solutions, colloids, and micellar systems by small-angle neutron scattering and inelastic scattering will require high-resolution instruments currently unavailable in the United States, including considerably more intense sources of cold neutrons. This research is essential for understanding how the properties of such systems are affected by the concentration, complexing agents, and constituents of the surrounding medium.

Biology and Medicine

Studies of the structure and dynamics of biological molecules and molecular assemblies will continue to be of major interest during the next decade. The use of neutrons and photons has provided much of the major understanding that we presently have of the molecular structure of biological substances, and continued development of these uniquely useful probes is essential.

The principal growth in the use of neutrons will be in the wavelength range from 3 to 20 Angstroms. Shorter wavelengths are appropriate for the study of macromolecular crystals at the atomic level. Good facilities for such measurements presently exist at the Brookhaven National Laboratory and at the National Bureau of Standards, although additional facilities and higher intensities would be welcome.

There is a major need for further instrumentation and development in the area associated with cold neutron research. This domain will include structural studies of macromolecular assemblies at low resolution, possibly through the use of crystals but certainly with solutions. Selective deuteration methods will be extensively used. Such approaches have been used successfully in studies of the structure of lipoproteins, ribosomes, nucleosomes, and DNA-dependent RNA polymerase from *E. coli*. The analyses of many other macromolecular assemblies

that may be amenable to neutron analysis now lie on the horizon, including studies of the RNA-protein complexes involved in processing messenger RNA and in controlling secretion. The higher-order structure of chromosomes is also of great interest and could be studied with neutrons of long wavelength.

Similarly, the study of biological membrane structure and the interactions of membrane components has provided a fertile area. Methodological refinements will permit a wider range of experimentation to probe both macromolecular interactions and membrane structures. Problems concerning the solvation of macromolecules, the formation of complexes between enzymes and substrates, and the interaction of ions with macromolecular surfaces are being pursued using scattering from solutions. Finally, recent applications of inelastic neutron scattering to macromolecules in solution suggest the possibility of obtaining fundamental thermodynamic parameters associated with macromolecular properties, and observing alterations in dynamic states that are correlated with functional changes in biological molecules. While this is a new area, success could lead to a greatly expanded use for inelastic scattering spectrometers that measure energy changes in the range from 0.01 to 100 meV. Thus, the needs for the coming decade in the neutron area are principally focused on the development and exploitation of instruments for cold sources.

Earth Sciences

Greatly improved energy-dispersive diffraction capability is required in the field of earth sciences. Here high-resolution diffraction of minerals at very high pressures, simulating geological stress conditions, is extremely important. Higher intensity pulsed sources will prove useful by permitting smaller samples and higher pressures to be employed. As in chemical crystallography, an order of magnitude increase in the flux from a steady state source would make it possible to greatly reduce required crystal sample volumes and open up a much larger number of mineral samples to investigation.

RESEARCH WITH MAGNET FACILITIES: PAST AND FUTURE

High magnetic field research is important for a fundamental understanding of a broad spectrum of material types and properties. Scientific advances in such diverse areas as superconductivity, permanent magnet research, and semiconductor science have all benefited from research based on the availability of intense magnetic fields. The attainment of such fields has, in general, been preceded by, and intimately connected with, applications developments and industrial commercialization. Each time a higher plateau of magnetic field strength is achieved, it is exploited quickly by the scientific community and is accompanied by the requirement for yet higher field strengths. The combination of high fields and low temperatures is

particularly important, along with ancillary measuring equipment such as that associated with precision optical measurements.

The Francis Bitter National Magnet Laboratory is the primary high magnetic field research facility in the United States. Direct current (dc) fields in the 20 tesla (T) range are available using Bitter magnets. To reach higher fields, hybrid magnets utilizing both superconducting and resistive coils are required. Using such procedures, the National Magnet Laboratory has achieved a steady state field of 30.4T. The ultimate limit for dc hybrid magnets appears to be 35 to 45T, beyond which pulsed magnetic field systems are needed. The National Magnet Laboratory currently offers nondestructive pulse systems to 45T. Higher pulse fields, perhaps up to 100T, appear to be achievable using advanced technology. In addition, the National Magnet Laboratory provides limited high-field, low-temperature facilities as well as high field facilities coupled with a variety of ancillary measurement equipment.

A great deal of progress in a number of areas has been made using relatively low fields, of the order of 1 to 2T, but the number and types of useful experiments that can be performed increase dramatically with higher field strengths. For example, the Zeeman splitting of a single electron in a field of 1T is the energy equivalent of only 1.4K. Increasing the field to 100T raises the splitting to 140K, which is comparable to typical exchange and crystal field energies in many magnetic systems. This raises the possibility of inducing large changes in the electronic structures and behavior of both magnetic and nonmagnetic systems simply by applying of such large fields. Some recent examples of exciting high magnetic field experiments are studies of the fractional quantized Hall effect at semiconductor interfaces, measurements of important superconductivity parameters such as H_c in materials that have significant technological applications, and the newly observed magnetic field induced charge-density-wave transition in graphite.

Clearly, the ready availability of higher magnetic fields could enhance measurements currently being made and create new research opportunities. A study by the NRC Solid State Sciences Committee conducted in 1979 but still valid today concluded (reference 3) that the availability of higher magnetic fields would open up many new, exciting, and profitable areas of research. The study found that one of the areas profoundly affected is that of semiconductor research. As a recent example, clear data elucidating the quantized sub-integer Hall effect have been obtained in experiments up to 28T and at ultra-low temperatures (50-100 milli K). Although not totally understood, these results are thought to arise from collective effects which suggest the possibility of additional phenomena to be investigated at even higher magnetic fields and with improved ancillary conditions. Among such physical phenomena might be unusual effects associated with charge density waves and, in the low density limit, Wigner crystallization. The latter possibility is particularly interesting for a high mobility two-dimensional electron gas that can be achieved in a selectively doped semiconductor heterostructure. Such an experiment would require the 2d electron gas to be in the high field limit in order to reduce

kinetic energy effects. Generally, such studies could have a major impact on improving our understanding of electron-electron correlation in an electron gas. Further, many of the techniques used to explore the electronic structure of semiconductors require that the cyclotron resonance frequency be high in comparison to the inverse scattering time of the electrons. For many materials, the scattering times are so short that this condition cannot be fulfilled with currently available magnetic fields. The only alternative in such cases is to go to higher magnetic fields. Other interesting phenomena in semiconductors that could be examined if sufficiently high magnetic fields were available include the breakdown in the effective mass approximation, electron-phonon "enhancement effects," and Zeeman splitting of deep impurity states.

Similarly, new scientific opportunities in metals and alloys emerge if intense magnetic fields are available. Many important metals and alloys have Fermi surfaces or parts of Fermi surfaces that cannot be measured at present, because either the effective mass or the electron scattering is too large. Both limitations could be surmounted in strong magnetic fields. Not only would it be possible to study the Fermi surfaces of exotic materials, but also of alloys well beyond the dilute limit. One might also envision measuring the Fermi surface of an alloy as it changed from the ordered into the disordered state. The age old problem of driving an exchange-enhanced paramagnetic system into the ferromagnetic state by applying a sufficiently large magnetic field might now be possible. Ferromagnetic Pd has not been found to date with the fields presently available. Increasing the upper limit for available magnetic fields might result in the induction of ferromagnetism in Pd.

The past several years have seen very exciting developments in the field of high-performance permanent magnet materials, especially new alloys based on the rare earth/iron/boron ternary compound, $Fe_{14}Re_2B$. The characteristics of these new materials for permanent magnets are based on large magnetization, very high magnetic anisotropy, and favorable microstructure. In a number of cases, such materials require magnetic fields in excess of 10T to achieve states near saturation. As improved materials become available, the field-intensity requirements may be even greater. The achievement of saturation fields is necessary not only in the production of permanent magnets, but in determining their fundamental properties from single crystal and oriented powder measurements. This provides a clear example of a field of research in which the availability of high magnetic fields could have a significant impact on major technological developments.

As discussed in the overview of this chapter, the study of superconductivity is the area of research that is most strongly linked to the production of high magnetic fields. Among materials currently being studied because of their interesting potential for use in high magnetic fields are the Chevrel phases, the B1 and A15 structures, as well as various types of thin film and inhomogeneous superconductors. High magnetic fields are also essential for probing those fundamental properties of superconductors that can be used to test microscopic

theories, such as those associated with certain types of electron pairing--singlet, triplet, etc.--as well as other basic features of high field superconductivity.

In addition to research areas involving high magnetic fields in a very fundamental way, there is a vast array of fields involving spectroscopic and other techniques that use high magnetic fields as a probe for extracting important information about the properties of physical, chemical, and biological systems. For many of these, such as nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), and the de Haas-van Alphen effect, the increased energy splitting available with higher magnetic fields provides tremendously enhanced ability to obtain information. At fields approaching 100T, energy splittings can also be great enough to have a direct effect on such phenomena as metallurgical phase transitions and chemical reaction rates. The ready availability of magnetic fields in these higher ranges would undoubtedly lead to a wide variety of applications and processes which utilize them in new and novel ways.

ADVANCED TECHNOLOGY NEEDS: APPLICATIONS OF NEW FACILITIES

The technological breadth of materials research can be sampled by looking at both the list of available applications in Table II.2 and the list of materials of economic importance in Table II.1. Technologically important examples have been described earlier in this chapter and are also given in numerous reports (references 1, 2, 3, 5, 6, 7, 8) dealing with synchrotron radiation, neutron scattering, and magnetic fields. Given below are examples of the connections between subareas of materials research and other fields which use major facilities and are linked to technological applications of national interest.

Semiconductors underlie all components involved in information systems--communication, computers, electronics. Techniques available at synchrotron radiation and neutron facilities are used to study structural and dynamic properties of semiconductors, including their interfaces, surfaces, and defects. X-ray scattering studies probe the atomic structure of semiconductors, while photoelectron spectroscopy techniques probe their electronic structure. Impurities of electrical importance in the range down to about 0.1 ppm or less, could be studied nondestructively using an x-ray microprobe on a new 6 GeV storage ring. High sensitivity, three-dimensional depth profiling of impurities and dopants in semiconductors and insulating films, can be studied with neutrons at concentrations down to 1 ppb if high-intensity cold neutron beams become available. X-ray lithography offers significant promise for fabricating precise submicron semiconductor structures for future VLSI applications. Doping by neutron transmutation is an essential tool for the production of semiconductor elements.

Essentially all other electronic materials, including metals, insulators, polymers, ceramics, and magnetic materials, can be characterized in unique ways using synchrotron radiation and neutrons. New structural and electronic properties of bulk and thin film materials,

as well as interfaces, defects, and surfaces can be studied in novel ways.

The use of special techniques is crucial if we are to obtain an understanding of the interfaces which lie at the heart of the devices used in modern electronics. In addition to providing knowledge concerning semiconductor interfaces, synchrotron-radiation-based surface science and neutron depth profiling are also useful in exploring interfaces at junctions of metals and insulators with semiconductors, both of which represent important physical features of modern electronic devices. In the future, more intense sources offer the ability to study the time dependence of surface and interface reactions, as well as opening up the possibility of developing microfocused beam techniques.

Extended x-ray absorption fine structure (EXAFS) has been widely used by industrial researchers to study materials. Examples involve the local atomic arrangements in alloys, specific impurity sites in coal, and active sites of catalysts. EXAFS spectra have been taken of a catalyst operating in a fuel cell. Future examples include the study of new materials produced by ion implantation, studies of the role of minority elements in alloys, and studies of composites.

Increased brightness from new sources will make it possible to use smaller concentrations and to follow changes on a more rapid time scale. Parallel studies with an x-ray microprobe will offer spatial resolution as well, so that grain boundaries can be studied. Scattering studies of complex materials like oil and structural materials are providing a microscopic understanding of such materials for the first time. As was the case in the electronics industry, such understanding will contribute significantly to future innovations in the energy industries.

The availability of facilities for SANS and high-resolution neutron spectroscopy has led to revolutionary advances in the understanding of polymers and many other materials in the past decade. The availability of more intense neutron sources will greatly expand the technological uses of SANS. For example, capabilities for high-sensitivity SANS will be needed to study in-situ microstructures that determine the strength and performance of lightweight, high-strength alloys and superalloys for airframe members and engine components in military aircraft.

SANS studies of voids and very small precipitates produced in pressure vessel steels under irradiation in power reactors will provide valuable information. High-intensity, long-wavelength SANS and large-angle diffraction studies of bulk ceramics during various stages of densification as well as in-situ characterization of microcracks, pores, etc., which affect their durability, will be possible. Such knowledge may, for example, be of potential use when ceramics are employed in automobile engines. Cold neutron SANS and high-intensity neutron spectroscopy techniques will be needed for in-situ studies of the porosity, molecular behavior and interactions in new catalysts and feedstocks that are employed in the production of chemicals and fuels. SANS instruments using cold neutrons will allow the probing of biological assemblies consisting of enzymes, nucleic acids, and lipids, which

control a large number of biochemical processes. These processes will often be relevant to biotechnological applications.

The unique characterization of materials with the use of high-intensity SANS will be available to study the polymeric constituents of new high-strength polymer blends and composites. This will include real time studies of phase separations related to processing. Such materials will provide increasingly important substitutes for heavier materials in autos, aircraft, and spacecraft.

Medical technologies are being advanced directly through the development of new diagnostic techniques. Moreover, the new light sources provide understanding at the microscopic level of many complex biological materials. A diagnostic example mentioned earlier is synchrotron radiation-based angiography. The study of platinum-based anti-cancer drugs by the EXAFS technique has provided clues to differences between effective and noneffective versions of these drugs. The production of medical isotopes using neutron sources will continue to be important in medical research, diagnoses, and therapy.

Synchrotron radiation and neutron facilities are important for the research programs of the defense agencies, both the Department of Energy and the Department of Defense. Advanced materials are of central importance to the defense agencies, which have needs ranging from information systems to structural materials involved in innumerable applications.

In a different class of application, remote sensors are employed in weapons tests, with particular emphasis on the hard and soft x-ray regions for diagnosis. Absolute absorption cross section spectra must be known, and detectors must be calibrated for such work. Both types of information can be obtained with the use of synchrotron radiation. While the temporal response of most detectors used in such work is faster than that of most synchrotron radiation sources, a next-generation storage ring will offer an improvement of about a factor of five.

There are several examples which illustrate the diverse applications of neutrons in research programs for national defense. High-intensity, energy-dispersive neutron diffraction is needed to measure local interaction stresses and textural characteristics which affect the performance of heavy metal shell components. Neutron depth profiling is needed to determine the tritium decay product (He^3) near the surface of refractory metals. High-intensity irradiation studies of metals and electronic components with fast neutrons are also essential.

In summary, the existing and proposed national facilities for materials research offer unique types of opportunities for both science and technology. It is difficult to think of significant issues affecting economic, defense, or health matters that cannot benefit in some essential way from the new opportunities presented by such facilities. This is, of course, the reason why they have already attracted the unparalleled participatory involvement of governmental and industrial research organizations. The new facilities considered in this report provide major opportunities for the next decade and beyond.

III. CONCLUSIONS AND RECOMMENDATIONS

The major facilities for producing synchrotron radiation, neutrons, and magnetic fields that are the focus of this report offer new opportunities essential for maintaining the progress and competitiveness of U.S. science and technology. These facilities will serve a broad spectrum of scientific fields, including materials research, biology, chemistry, atomic and molecular physics, plasma physics, the earth sciences, and medical science. As unique facilities offering incomparable scientific and technical opportunities, they will enable scientists and engineers to pursue otherwise inaccessible areas of science and technology. They will affect the technologies of information and defense, as well as those of energy, transportation, and health.

Materials research is the principal field served by these facilities. However, within this multidisciplinary field, there are also important research areas that are best served by specialized instruments of moderate cost that can be placed under the control of a single investigator or small group of investigators. Such research will often continue to be addressed most effectively by the Materials Research Laboratories and other relatively small and specialized research teams sharing comparatively small facilities, of the type described in Chapter I. Indeed, most of the research goals that the major facilities are expected to address originated through the insights of "small science" and will often be pursued jointly with groups also involved in small science.

The major materials facilities now operating—including those for neutron scattering, those for the production of synchrotron radiation, and the National Magnet Laboratory—are essential parts of the research effort of the United States. In some cases, these existing facilities will be superseded by new ones with additional capabilities. It will, however, be several years, and in some cases more than a decade, before the major new facilities recommended in this report can contribute directly to the national research effort.

The Committee emphasizes that its recommendations for major facilities--both new facilities and new capabilities at existing ones--embody two important prerequisites:

- That they are accompanied by expanded support of smaller materials research programs, including related instrumentation. Research on this scale continues to provide much of the fundamental new science in the field and to train a large fraction of our scientific and technical manpower.

- That resources must be provided to operate existing user facilities productively. In addition, the approved enhancements of major synchrotron radiation facilities at the Brookhaven National Laboratory, Stanford University, and the University of Wisconsin should be completed expeditiously, since it will require from several years to more than over a decade before the new facilities recommended in this report can contribute to the research effort of the United States.

RECOMMENDED PRIORITIES

The Committee's recommended priorities for the development and construction of facilities during the next decade include two categories:

- Major new facilities, and

- New capabilities at existing facilities.

These two categories complement one another in function, time and required resources. New capabilities at existing facilities are essential for scientific and technological needs during the next decade. The period from five years to more than a decade needed to construct major new synchrotron radiation and neutron facilities require that we start now in planning and designing these facilities. As discussed in Chapter II, failure to proceed with such new facilities will have an adverse and enduring impact on many fields of science and technology, diminishing the nation's competitive standing in such fields. The Committee concludes that both new facilities and new capabilities at existing facilities are essential for the effective evolution of science and advanced technology in the United States in the next decade and beyond.

The Committee also recommends the convening of additional panels to address other important aspects of materials research.

Major New Facilities

The Committee's recommendations for the construction of major new facilities are listed below in order of priority. A brief description and rationale is given for each recommended facility.

1. A 6 GeV Synchrotron Radiation Facility. This facility would effectively exploit the new scientific and technological opportunities made possible by insertion devices. These devices, by producing synchrotron radiation having orders of magnitude greater brightness than is currently available, would make it possible to expand on the seminal research using synchrotron radiation of the past decade. The first generation of storage rings designed as synchrotron radiation sources is now becoming operational, i.e., the National Synchrotron Light Source, at Brookhaven, and the Synchrotron Radiation Center, at the University of Wisconsin. While they will provide important capabilities, concurrent advances in design make it possible to construct storage rings and insertion devices with orders of magnitude improvement in brightness. A 6 GeV synchrotron radiation facility exploiting such advances offers both identifiable and as yet unforeseen opportunities for research not possible at present facilities.

This 6 GeV ring would have many long, straight sections containing insertion devices--undulators and wigglers. The storage ring would be designed to provide an electron beam that optimizes the emittance or intensity, or both, of synchrotron radiation from the insertion devices. A storage ring of about 6 GeV is optimal for producing undulator radiation in the 10 keV region where most x-ray research is done. The radiation from such a source would be orders of magnitude brighter than from any existing dedicated source. Wigglers on such a ring can provide unmatched intensity over a wide spectral region. The time-dependent characteristics of the radiation--short pulse length and long inter-pulse times--would make it at least as useful as that from existing sources. Moreover, insertion devices for the production of soft x-ray and vacuum ultraviolet radiation in the range from 100 eV to 1 keV would yield a thousand-fold brighter radiation than any source now operating, although not as bright as those possible on a new 1 to 2 GeV ring (Priority 3).

Timely construction of a 6 GeV synchrotron radiation facility would give the United States continued leadership in this important and dynamic field. Site-independent design should begin immediately, and the choice of site and construction should commence as soon as possible. If construction begins, for example, in FY 87, operation is possible by FY 92.

2. An Advanced Steady State Neutron Source Facility. The goal is to achieve about ten times the flux of existing machines with a minimum requirement of five times the flux. There are two principal reasons for the priority.

First, and most important, a new high-flux source can be designed to optimize beam geometry and flux distribution, so as to yield increased intensities for all experiments. An increase of about ten

times the flux of existing machines is an aggressive but technologically feasible goal. Neutron scattering is inherently a signal-limited technique. The new facility would greatly increase the range of neutron experiments in materials research and other fields, as well as the precision with which relevant energies and momenta could be measured.

Such a neutron source would ensure the United States a leading position in this field, especially in the cold neutron range, where flux increases of an order of magnitude can be achieved. Such increases offer new capabilities, for example, in high resolution spectroscopy and studies of small angle scattering.

Second, the current high-flux reactors in the United States were all commissioned in the 1960's, so that there are significant concerns about their long-term viability. Given that design and construction of a new facility will require about a decade, planning must begin now to furnish needed capability for the late 1990's and beyond.

The Committee suggests that the design and construction of a new facility include the following: (a) at least one large guide hall containing many large-area guide tubes for cold and thermal neutrons; (b) a reactor hall containing many thermal beams, along with several "hot source" beams for high-energy neutron research; (c) a variety of spectrometers, including many with new capabilities beyond present designs; and (d) improved national facilities for isotope production, irradiation of materials, neutron activation analysis, and research in nuclear physics.

Instead of upgrading an existing reactor, a new facility should be built, and site-independent design should begin immediately. Because of the complexity of safety requirements, the Committee does not expect construction to begin until about FY 89, with completion possibly by FY 96.

3. A 1 to 2 GeV Synchrotron Radiation Facility. The Committee has concluded that, while the 6 GeV storage ring can furnish important new capabilities for the lower-energy region, a single such facility may not provide adequately for the national opportunities of the next decade. Among the reasons for this are: (a) the optimum storage ring energy for producing fundamental undulator radiation with wavelengths in the range of 10 Angstroms and greater is about 1.5 GeV, a region offering special opportunities for research in chemical physics and electron spectroscopy; (b) in addition to an increase in brightness, the unwanted total power density associated with a 1 to 2 GeV ring is significantly lower at wavelengths longer than 20 Angstroms; and (c) the undulator radiation from a 1 to 2 GeV source will have a higher degree of coherence than that from undulators elsewhere, thereby opening opportunities to apply various imaging techniques, such as microscopy and holography. A 1 to 2 GeV facility would provide optimal flexibility for both VUV and soft x-ray users.

This facility, then, would be centered around insertion devices but optimized for high brightness in the soft x-ray and VUV synchrotron radiation regions. The growth of research using these spectral regions has paralleled that in the x-ray region. Moreover, major advancements in design have occurred, permitting large increases in brightness for such a source.

4. A High-Intensity Pulsed Neutron Source Facility. Pulsed neutron facilities offer the best capability for sources of high-energy neutrons and the most promising approach to future advances beyond those that appear possible with steady state sources. In the few years that pulsed sources have been available, they have led to innovative research using new time-of-flight techniques and have served a broad user community, even though limited to modest peak fluxes.

The new capabilities recommended at existing facilities, for example, the attainment of a 10^{16} neutrons/cm^2-sec peak flux at the Los Alamos National Laboratory facility—Priority 3 in new capabilities given below—are expected to advance research using pulsed neutrons even further. Action on the design and construction of a pulsed source with a peak flux in the range of 10^{17} neutrons/cm^2-sec should be based upon the results obtained from such new capabilities.

New Capabilities at Existing Facilities

The Committee's recommendations for adding new capabilities at existing facilities are listed below in priority order. Brief rationales and descriptions are given for each recommendation.

1. Centers For Cold Neutron Research. Guide halls and instrumentation for exploiting the only cold neutron sources in the U.S., located at the Brookhaven National Laboratory and the National Bureau of Standards facilities, should be developed in an orderly fashion.

These facilities are urgently needed to address the rapid expansion of neutron applications in materials science, chemistry, and biology; many central problems in those fields can only be solved using new instruments with cold neutron beams. These centers will provide a diverse, flexible array of cold neutron instruments, matching current capabilities in other industrialized nations. Further, by using advanced techniques for beam focusing and polarization, such facilities would exceed existing worldwide capabilities, in areas such as high resolution spectroscopy of catalysts and polymer systems and in studies of impurities and inhomogeneities in bulk materials.

Research using cold neutron facilities has received inadequate support in U.S. during the last decade, a period of major investments in cold neutron research in other countries. The Western European investment alone is at least ten times that of the United States. There are only two cold neutron reactor sources in the United States one at Brookhaven and one being developed at the National Bureau of Standards. Guide halls, which improve the versatility and flexibility of cold or thermal neutron instruments, do not exist in the United States while there are six fully instrumented cold neutron guide halls either completed or under development in Western Europe. Implementing this priority will enable U.S. scientists to be competitive in cold neutron research during the next decade and will provide new instrumentation concepts for developing future neutron scattering facilities.

2. Insertion Devices on Existing Facilities for Synchrotron Radiation. Insertion devices and instruments should be developed in an orderly fashion to exploit about six of the remaining straight sections

of existing storage rings. The special characteristics of undulators as radiation sources should be emphasized, since they enable new capabilities not available presently at existing facilities.

Existing storage rings fitted with insertion devices will be our premier sources of synchrotron radiation for the next 5 years or more, or until new facilities described in this report are completed. Further, they will provide valuable experience for designing and implementing our next generation of synchrotron radiation facilities.

There are, currently, only four operational insertion devices, all wigglers. Nine new insertion devices have been proposed and approved for funding, of which only three are undulators. This number of insertion devices is clearly inadequate to meet future national needs and requires the development and implementation of additional devices.

Thus, the construction of additional insertion devices, when it is approved, should follow the construction of new capabilities at synchrotron radiation facilities already included in the budgets for FY 85 and FY 86.

3. Experimental Hall and Instrumentation at the Los Alamos National Laboratory. An experimental hall and new instruments at the Weapons Neutron Research/Proton Storage Ring (WNR/PSR) pulsed neutron source at the Los Alamos National Laboratory (LANL) would make the United States competitive in pulsed neutron research and would help guide the development of future pulsed sources. The expected flux increase at this facility provides an important opportunity to explore, at modest cost, the great promise of pulsed neutron science in relation to spectroscopic and structural problems. Although this technology is young, the instruments developed at the Argonne and Los Alamos national laboratories demonstrate that innovative approaches can produce enhanced capabilities.

Pulsed sources are superior to steady state sources in generating neutrons of short wavelength. It also appears that instruments for pulsed sources can be developed that will be advantageous at long wavelengths in certain cases. Developing the new source at the WNR/PSR at Los Alamos should, for a relatively modest investment, provide an important new tool for research and also permit a detailed assessment of the best course for developing future pulsed sources. Overall, the Committee feels that the WNR/PSR facility should be exploited fully. In considering the specific opportunity at Los Alamos, important factors taken into account were the peak intensity that could be attained (greater than 10^{16} neutrons/cm^2-sec), the relative economy of the investment, and the speed with which the facility could become operational.

4. Upgrade of the National Magnet Laboratory. The National Magnet Laboratory (NML) is the only high magnetic field user facility in the United States. Many areas of materials research require combinations of high fields and/or low temperatures. Both the 45T pulsed field system and the 19T/50 mK system at the NML require enhanced instrumentation to permit full exploitation. The position of NML as the leader in magnetic field research depends on the timely development of a new hybrid system that will provide higher fields at lower cost for a rapidly growing community of users. Additional funds are needed to

complete the project. A pulsed magnetic field system capable of 75T could also be placed on line more quickly with adequate funding. Recent experience shows that even modest increases in magnetic field capability can open new approaches for addressing important problems in condensed-matter science and increase the demand for NML facilities significantly.

5. Enriched Pulsed Neutron Source Target. Enriched targets exploit higher levels of fission to amplify the production of neutrons and can more than double the available flux. Such increases in flux are important because neutron scattering is inherently a signal-limited technique. The development and installation of enriched targets for use at pulsed neutron facilities would be cost effective.

Priorities 1 and 2 for major new facilities, when they are implemented, would serve as a centerpiece of this nation's future capability for synchrotron radiation and neutron based research. Thus, design and siting studies for a 6 GeV synchrotron radiation facility and for an advanced steady state neutron facility should begin immediately.

Because of the long lead time associated with an advanced steady state neutron facility, the immediate implementation of at least one instrumented cold neutron guide hall is necessary to provide forefront capability.

ESTIMATED COSTS OF THE RECOMMENDATIONS

To summarize the overall scale of its recommendations, the Committee presents, in Table III.1, its estimates of the requirements for new funding in millions of FY 85 dollars. The estimates in Table III.1 include costs of construction and initial instrumentation for major new facilities and new capabilities at existing facilities. Estimates for major new facilities assume initial instrumentation for one-half of the available beam line capability.

There are also additional costs associated with the development, maintenance, and scientific use of these advanced facilities. The Committee estimates related personnel costs to be about $250 thousand per year for each neutron or synchrotron end station. The same is true for major new magnetic field stations. A somewhat smaller amount is required for other experimental purposes and/or instrument maintenance. More detailed information can be obtained from the presentations included in the supplemental volume to this report. In addition, there will obviously be some incremental travel, subsistence, and experimental costs for the hundreds of scientists and engineers who will use these new facilities, costs which may be covered only in part by reassignment of funds used for other scientific purposes.

Table III.1 REQUIREMENTS FOR NEW FUNDING*

MAJOR NEW FACILITIES (Millions of FY 85 Dollars)

In order of priority:

1.	6 GeV SR Facility	$ 160
2.	Steady State Neutron Source Facility	260
3.	1 to 2 GeV SR Facility	70
4.	High Intensity Pulsed Neutron Source Facility	330

NEW CAPABILITIES AT EXISTING FACILITIES (Millions of FY 85 Dollars)

In order of priority:

1.	Centers for Cold Neutron Research	$ 25-35 each
2.	Insertion Devices on Existing SR Facilities	20
3.	Experimental Hall and Instrumentation at LANL	15
4.	National Magnet Laboratory Upgrade	5
5.	Enriched Pulsed Neutron Target	2-5

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* The Committee's estimates for construction and initial instrumentation costs are largely based on information from facility presentations, program officers, and other knowledgeable colleagues.

Major New Facilities

1. The new 6 GeV synchrotron radiation facility has an estimated cost of $160 million, including $125 million for construction and $35 million for instrumentation. The instrumentation would equip fully about 10 insertion devices, and associated beam lines, with about 20 experimental end stations. The estimated operating cost is about $20 to $25 million per year.
2. The new steady state neutron source has an estimated facility cost of $260 million, including $220 million for construction and $40 million for about 20 instruments. The estimated operating cost is $12 million per year.
3. The 1 to 2 GeV synchrotron radiation facility is estimated to cost $70 million, including $50 million for construction and $20 million for the instrumentation of 6 instrumented beam lines with about 12 end stations. The estimated operating cost is $9 million per year.
4. The high-intensity pulsed neutron source facility is estimated to cost $330 million, including $310 million for construction and $20 million for instrumentation of about 15 instruments. The estimated operating cost is $25 million per year.

New Capabilities at Existing Facilities

1. The centers for cold neutron research would cost $25 to 35 million each, about half for guide hall construction and half for instrumentation. The instrumentation funding would provide up to 20 cold neutron instruments and associated equipment. There are no incremental operating costs for the reactor associated with these new capabilities.
2. Insertion devices on existing synchrotron radiation sources would cost about $20 million for 6 fully developed lines, including about 12 x-ray and VUV instruments. There are no incremental operating costs for the associated synchrotron sources.
3. The experimental hall and instrumentation at the Los Alamos National Laboratory would cost $15 million and provide a large area for the installation of more than 10 instruments, 3 of which would be funded as part of the LANL proposal. Additional pulsed source operating costs of $2.7 million per year are required.
4. The National Magnet Laboratory upgrade requires about $5 million.
5. An enriched pulsed neutron target would cost between $2 and 5 million. Operating costs for the source would increase between $0 and 0.7 million.

Current major facilities will likely be superseded by the new facilities in certain cases, and their operating cost budgets will be transferred. An example is given by the steady state neutron source, whose construction could result in the phasing out of one of our current sources. This, in turn, would have the effect of requiring only a slight increase in net operating costs for the new facility.

The Committee considered possible funding schedules for each of the foregoing recommendations. In general, the new capabilities at

existing facilities can be implemented within about 3 years from initial funding, whereas the major new facilities are estimated to require construction times from about 5 years to as long as 10 years.

In response to its charter, the Committee has determined the order of priority of construction of new facilities that are important for the rapid and effective progress of materials research and related fields. We show in Figure III.1 an estimated funding profile for design and construction associated with an expeditious implementation of all the items in these priority lists except for the 10^{17} neutrons/cm^2-sec pulsed neutron source facility, whose starting date is uncertain. The Committee does not necessarily recommend that all priorities be funded at the respective times indicated. The diagram is intended to suggest the approximate earliest possible start dates and construction time intervals for the various priorities. We note that accurate estimates of both construction costs and time schedules can only be obtained from specific proposals from specific institutions. The funding profile for priority 2 shown in Figure III.1b extends from fiscal years 1987 to 1989. Under this schedule, priority 2 modifications would follow the completion of those new capabilities at existing synchrotron facilities that are already included in the budgets for fiscal years 1985 and 1986.

With the foregoing in mind, several important general conclusions can be deduced from Figure III.1. First, implementation of new capabilities at existing facilities is complementary in time to the implementation of major new facilities. Second, with modifications of schedule, a relatively flat funding profile of construction is possible over the next decade, with an average expenditure rate of roughly $50 million per year for about a decade if all priorities are implemented. Third, the total construction fund of $588 million appearing in Figure III.1 is roughly comparable, in FY 85 dollars, to the average total U.S. capital investment per decade over the past two decades to provide facilities for synchrotron radiation, neutron production, and high magnetic fields, namely, in the range of $300 million, $500 million, and $20 million, respectively.*

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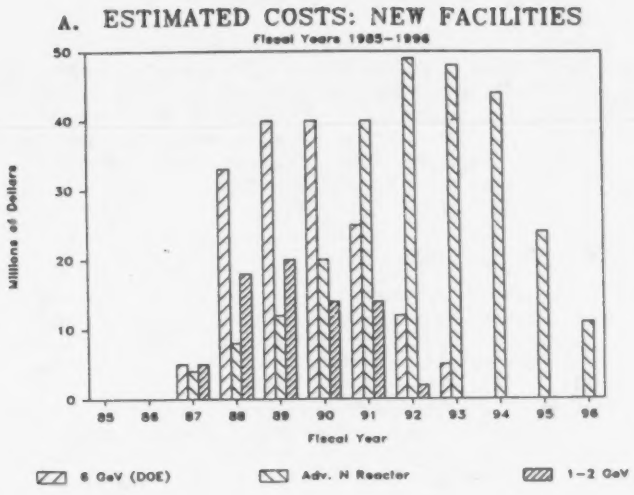
* The replacement costs in FY 85 dollars for existing multi-purpose neutron sources and related major instrumentation built over the past 20 years (primarily in the 1960's) is of the order of $500 million. This includes, for example, the HFIR at Oak Ridge, the HFBR at Brookhaven, the NBS reactor, the University of Missouri reactor, and the intense pulsed neutron source at Argonne. A comparable figure for synchrotron radiation sources and associated instrumentation (primarily developed over the past decade) is estimated at about $300 million including facilities at Brookhaven (NSLS), Stanford (SSRL), Wisconsin (Aladdin, Tantalus), Cornell (CHESS), and NBS (SURF II). Estimates for the synchrotron radiation facilities includes the construction cost of SPEAR at Stanford but does not include any share of other accelerator facilities used in a parasitic mode for synchrotron radiation at Cornell and Stanford.



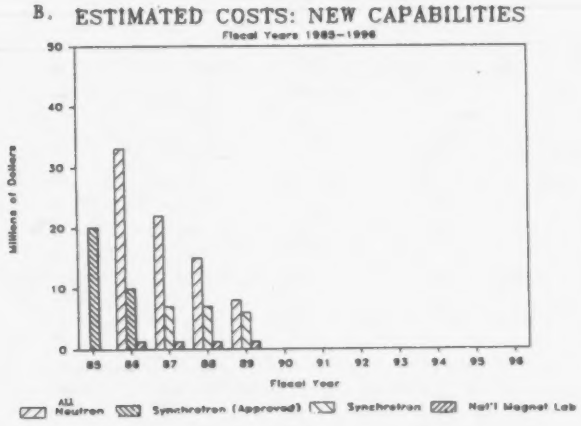


FIGURE III.1. Estimated Costs Versus Year. Estimated costs and earliest possible schedules for construction and initial instrumentation of (a) a 6 GeV synchrotron radiation facility, an advanced steady state neutron source, and a 1-2 GeV synchrotron radiation facility and (b) all recommended priorities for new capabilities at existing facilities.

The funding profile for priority 2 shown in Figure III.1b extends from fiscal years 1987 to 1989. In this schedule, modifications associated with priority 2 would follow the completion of those new capabilities at existing synchrotron facilities that are already included in the budgets for fiscal years 1985 and 1986. The Committee does not necessarily recommend that all priorities be funded at the respective times indicated.

OTHER SPECIALIZED FACILITIES CONSIDERED BY THE COMMITTEE

In addition to facilities for synchrotron radiation, neutron scattering, and high magnetic fields, the Committee surveyed other major facility needs and opportunities during the course of its study. However, none was identified that qualified for the priorities under the guidelines, namely $5 million minimum cost, established by the Committee's charter. We summarize here the specific items considered and the reasons for excluding them from detailed considerations.

Medium-Scale Specialized Facilities

The Committee briefly considered interdisciplinary materials research organizations, such as the Materials Research Laboratories (MRL) funded by the NSF and DOE, as well as special-purpose materials research laboratories or such centers for materials research as those on polymers, ceramics, and materials processing and other focused sub-areas of materials research. The Committee believes that such laboratories and centers represent a very important part of our overall national materials research program and that they fulfill national needs not otherwise satisfied by academic, governmental, or industrial laboratories.

The Committee heard excellent arguments for new facilities of this type, each of which can easily cost more than $5 to 10 million. However, the Committee excluded consideration of them without prejudice. It did so in part because of their "open-ended" nature. They require fuller definition through the formulation of specific proposals by specific institutions. The Committee did not request development of the details of such proposals when they were not already well formulated. Further considerations of important materials research laboratories and centers are deferred for future planning committees.

The Committee also discussed facilities for developing microelectronics processes. These are rapidly gaining national importance as microelectronic technology reaches submicron levels in silicon, and as materials other than silicon, such as gallium arsenide, are explored. Most large-scale facilities for microelectronics processing have, quite appropriately, been established by industry, though there is also a role for universities in this area.

Also discussed were facilities for high and ultra-low temperatures as well as those involving charged-particles such as electron microscopes and ion beam facilities, which can make major contributions to the analysis, synthesis, and modification of materials. The individual costs of these generally fall below the $5M threshold used by the Committee. As a result, and without passing any judgment on relative merits, such facilities would be better considered as part of the analysis of serious instrumentation needs mentioned earlier in this report. Such instrumentation will play important roles in conjunction with the use of synchrotron radiation sources, in which case their costs will be included along with those of beam lines.

Specialized Photon Sources

The Committee examined various other photon sources, such as high peak-power VUV excimer/dye-laser schemes, transition-radiation and bremstrahlung sources driven by intense relativistic electron beams, free-electron lasers, and soft x-ray sources derived from laser-heated plasmas. VUV laser sources based on nonlinear mixing of excimer and tuneable dye lasers were judged very promising. This technology deserves rapid development. The facility costs for such sources, although quite substantial when judged by traditional academic research standards, are expected to fall considerably below the Committee's $5 million threshold. Practical realization of the other photon sources listed above would require large capital investments.

However, only the free-electron laser appears to be of general interest at this time when employed in a user mode, because of its high brightness and broad tunability. This technology is currently under active development at many laboratories, both in the United States and abroad. The eventual utilization of free-electron lasers operating in the infrared seems a certainty. Efforts should be made to stimulate the establishment of a user community. The practical short-wavelength limit of such systems is not yet known, although operation of such lasers to 50 nm (5 nm with harmonic generation) has been projected. Considerable development effort is needed, particularly with regard to high-reflectance mirrors in this spectral region. Although it is premature to rank the value of free-electron lasers, they may eventually prove to be extremely important at photon energies in the range of 10 to 100 eV, and thus complement VUV/soft x-ray synchrotron radiation sources.

Computation Facilities

As indicated in Chapter I, the Committee also made an effort to examine the growing importance of large-scale computational support in the materials sciences. Theoretical materials science has now reached a point where, given adequate computer support, it can predict with quantitative accuracy, typically 1 to 10 percent, the physical properties of many materials systems, and thus complement experimental approaches.

The most effective kind of computer support for the national materials science community therefore is provided by a combination of a national network of Class 6 supercomputers and a number of smaller computers that are used by local or regional groups. The Committee strongly supports a major initiative in this direction now being undertaken by the National Science Foundation. It also strongly supports plans of the Department of Energy to extend the availability of networked supercomputers to scientists working in other areas. It hopes that other agencies supporting basic research will also take appropriate actions.

Muon Facilities

Pulsed muon beams, derived parasitically at high-energy particle accelerators, have received considerable attention for studies of condensed-matter physics that are based on measurements of spin-rotation. Several centers which support such research currently exist, and modest growth is anticipated. Some thought is being given to a major dedicated beam line at the Los Alamos LAMPF proton storage ring. The cost for such an addition may reach $30 million. It appears premature to judge the merit of such a facility, given the currently small size user community and the highly specialized nature of the technique.

Engineering Materials Test Facilities

Facilities in this category cover a very broad range with respect to the physical parameters studied and the associated capital costs. Major needs of this type for which federal, rather than industrial, funding is appropriate are primarily linked to mission oriented programs, such as national defense. As a result, they are not under the purview of the Committee.

Facilities Only Peripherally Related to Materials Science

Facilities whose principal purpose is not related directly to materials science were not considered by the Committee. An example is the proposal at Sandia for a Combustion Research Center (Phase II). The central thrust of this proposal is directed toward combustion science and technology. The behavior of materials at combustion temperatures is only one among a large number of other important topics projected for investigation at this laboratory as part of the new initiative.

National facilities for research in the physics of condensed matter

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(Received 21 October 1983; accepted for publication 15 November 1983)

Brief descriptions are given of 23 national facilities in the U. S. that are of importance to research in the physics of condensed matter. These facilities range from nuclear reactors and synchrotron sources to high-voltage electron microscopes and facilities for the preparation of special materials and submicron structures. They take a variety of forms and are located in several kinds of institutions, but are alike in being available to qualified scientists from other laboratories. The primary purpose, size, major experimental equipment, and method of operation are described for each facility.

PACS numbers: 29.25.Dz, 61.90. + d, 07.80. + x, 89.20. + a

INTRODUCTION

At the American Physical Society meeting in Los Angeles in March of 1983 an invited poster session was held on National Facilities of Importance to Condensed Matter Physics. The session was arranged by the Division of Condensed Matter Physics. There were 23 facilities featured, ranging from nuclear reactors and synchrotron sources to high-voltage electron microscopes and facilities for the preparation of unique materials or submicron structures. Most of the facilities on display have come into operation within the last five years, many within the last one or two. This fact reflects the rapid increase in the importance of large research devices and combinations of large devices in condensed matter physics, together with the necessity that, because of their cost such facilities be developed on a national basis and widely shared. Thus a pattern of usage is developing in condensed matter physics which has been common in particle physics for many years, and institutional arrangements are evolving for accomplishing this objective effectively and fairly. All these central facilities are governmentally funded. Only two, however, are operated directly by the federal government; the others are operated by contractors, many in national laboratories, some in state universities.

Even though the 23 facilities included all of the very large national facilities which are of prime importance to condensed matter physics, the display was not exhaustive. Other facilities exist that were not included because of space limitations. The list, however, gives an excellent view of the present national posture. It shows that the United States is in a strong position, but also makes it clear that condensed matter physics is a dynamic area in which rapid growth and frequent change must occur. It is hoped that this review will be valuable to potential users and will assist in the wide dissemination of information on what is available and how the interested researcher goes about gaining access to these centers.

It is evident that a strong trend toward national user facilities is still in full swing, and that more centralized facilities for condensed matter research will soon become available. Decisions on what new centers are most needed should be aided by this overview of what exists now.

In the following, a short synopsis of each facility is given, including its primary purpose, major equipment, size, and method of operation. Sources from which one can obtain more information are also provided.

The facilities are grouped under the following headings: (1) neutron sources; (2) synchrotron radiation sources; (3) facilities for microanalysis, microfabrication, and surface studies; (4) electron microscopes; and (5).

The writers are indebted to the operators of the various facilities for their cooperation in supplying information.

I. NEUTRON SOURCES

Nuclear reactors have been the traditional sources of neutron beams for condensed matter physics since the 1940's. Four U. S. reactors which are national facilities are described in this section. Also included is a facility within a facility, the National Center for Small Angle Scattering Research at Oak Ridge.

More recently pulsed neutron sources driven by medium energy accelerators have come on the scene, and two of these which are now national facilities are represented.

The main focus in what follows is on neutron scattering; radiation damage in materials has not been emphasized. Most of these facilities, however, also offer capabilities for exposing specimens to various kinds of radiation.

A. High Flux Beam Reactor, Brookhaven National Laboratory, Upton, NY

The High Flux Beam Reactor (HFBR) provides the scientific community with one of the most intense thermal neutron sources in existence today. The HFBR began operating in 1965 at a power of 40 MW. It has had a cold neutron

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facility with liquid-hydrogen moderator operating since April 1981. The reactor was recently upgraded and has been operating at 60 MW since September 1982. Many types of experiments are possible at the HFBR, including magnetic and nonmagnetic structure studies, phonon and magnon dispersion measurements, and diffuse scattering studies. Because of the relatively high energy resolution and the sensitivity of neutrons to magnetic moments and to the nuclei of almost all elements of the periodic table, neutron scattering makes feasible many studies which would be difficult or impossible with x rays. Facilities of interest to solid-state physicists at the HFBR include several triple-axis neutron spectrometers which can be used for both elastic and inelastic scattering measurements with incident neutron energies between 2 and 200 meV. A wide variety of different sample environments is available, including temperatures from 35 mK to 1500 K, magnetic fields up to 7 T, and pressures up to 35 kbar.

For additional information contact B. H. Grier or G. Shirane, Physics Department, Brookhaven National Laboratory, Upton, NY 11973.

B. High flux isotope reactor, Oak Ridge National Laboratory, Oak Ridge, TN

The High Flux Isotope Reactor serves the condensed matter physics community by providing high-intensity beams of thermal neutrons. The scattering facilities available include eight different instruments, not counting the 30-m Small-Angle Neutron Scattering (SANS) instrument described elsewhere. They are: (1) the triple-axis polarized-beam spectrometer, which permits polarization analysis experiments; (2) and (3) two general-purpose triple-axis spectrometers used for most of the phonon dispersion measurements, but which are also useful for modest resolution quasielastic studies and fairly high resolution powder diffraction studies; (4) a liquid diffractometer with a linear position-sensitive detector; (5) a double perfect-crystal, very-high-resolution SANS spectrometer which has been used primarily to study vortex lattices in superconductors; (6) a four-circle diffractometer for crystallographic studies; (7) a more limited triple-axis unit with a fixed incident energy of 14.7 meV; and (8) a time-of-flight correlation chopper spectrometer. The latter has been equipped recently with a system of ultrasonically pulsed silicon crystals to monochromatize and pulse the neutron beam incident on the sample.

A new two-dimensional detector has been developed; it utilizes a 12-in.-diam neutron-sensitive LiF–ZnS phosphor, an image intensifier, and a television camera system. This detector has been extremely useful in the observation of diffuse scattering, superlattice formation, and powder patterns, as well as crystal characterization, all in real time (less than a second). The system also has image storing capabilities.

Some of the auxiliary equipment includes furnaces, closed-cycle refrigerators, helium-four cryostats, a helium-three cryostat, a superconducting magnet, and a helium-three–helium-four dilution refrigerator with a split-coil superconducting magnet, which is capable of reaching 7 mK and a field of 5 T.

For additional information contact H. A. Mook, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830.

C. Research reactor facility (MURR), University of Missouri, Columbia, MO

The University of Missouri operates a 10-MW reactor as a neutron and gamma radiation source for condensed matter research. Interested parties from outside the University are encouraged to make use of the facility through cooperative experiments with members of the staff, or through the Reactor Sharing Program, supported by the Department of Energy. At MURR there are facilities to conduct experiments in at least four areas related to condensed matter physics research. (1) For neutron scattering, two triple-axis spectrometers are available to measure dispersion relations; two single-crystal diffractometers and one powder diffractometer are available to measure atomic and magnetic ordering in condensed matter systems; one small-angle neutron scattering spectrometer is available for polymer and molecular biological studies; a neutron interferometer can be used for special experiments. (2) For gamma scattering, three unique instruments are available: MUGS, which is a gamma-ray diffractometer for structure studies; QUEGS, which is a gamma diffractometer with Mossbauer energy analysis for quasielastic gamma measurements; and COGS, which is a Compton spectrometer now available for measuring momentum distribution of electrons. (3) Trace element analysis can be done by instrumental, radiochemical, and prompt neutron activation; it allows the characterization of elements in condensed matter samples. (3) Analyses of deep levels in the band gap of semiconductors can be made by using deep-level transient spectroscopy, current transient spectroscopy, and the newly developed charge transient spectroscopy, which allows 10^{10} deep levels per cubic centimeter to be detected.

For additional information contact R. M. Brugger, Director, Research Reactor Facility, Research Park, Columbia, MO 65211.

D. NBS research reactor, National Bureau of Standards, Gaithersburg, MD

The NBS research reactor is expected to double its power to 20 MW by the end of 1983. In March of 1983 it had 25 experimental facilities installed for materials reseach, activation analysis, radiation standards, and nuclear physics. Ten of the horizontal beam ports are dedicated to condensed matter science, with a wide variety of neutron scattering instruments installed. Special features include: (1) a three-axis spectrometer with two low background analyzer systems to allow measurements ranging from soft modes and spin-wave excitations in solids (as low as 1.0 meV) to the spectroscopy of low levels of hydrogen and molecular species in metals and catalysts (30–300 meV); (2) a multidetector high-resolution diffractometer used to study complex structures by powder diffraction, e.g., magnetic intermetallic compounds, catalysts, and ionic conductors; (3) a biological diffraction station used to study the structure of proteins; (4) a depth profiling facility for the nondestructive determination of density profiles of selected elements near surfaces; and (5) a small-angle neutron scattering facility with continuously variable wavelengths from 4 to 10 Å, a wave vector transfer

range from 0.003 to 1.0 $Å^{-1}$, and on-line color graphics for the study of microstructure in metals, polymers, and biological materials.

For additional information contact J. J. Rush or J. M. Rowe, National Bureau of Standards, Washington, DC 20234.

E. National Center for Small-Angle Scattering Research, Oak Ridge National Laboratory, Oak Ridge, TN

The National Center for Small-Angle Scattering Research is a user-dedicated facility supported by the National Science Foundation and the Department of Energy under an interagency agreement. The two main instruments available to users are the NSF-supported 30-m small-angle neutron scattering facility (SANS) and the DOE-supported 10-m small-angle x-ray scattering camera (SAXS). These instruments are intended to provide state-of-the-art capability for investigating condensed matter structures in a range from a few tens up to several hundreds of angstroms. They are intended to serve the needs of scientists in the areas of biology, polymer science, chemistry, metallurgy and materials science, and solid-state physics.

For additional information contact W. C. Koehler, Director, or M. Gillespie, Secretary, NCSASR, Oak Ridge National Laboratory, Oak Ridge, TN 37830.

F. Intense Pulsed Neutron Source, Argonne National Laboratory, Argonne, IL

The Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory (ANL) is the most intense neutron spallation source now operating in the world. Protons from a 50-MeV linear accelerator and a 500-MeV rapid cycling synchrotron are delivered to a uranium target at a frequency of 30 Hz to produce neutrons. In the first year of operation 3370 h of research time were available. The peak thermal flux of IPNS is 3×10^{14} n/s cm^2.

The instrument package at IPNS has been designed with particular attention to the rich epithermal spectrum of neutrons present in such a spallation source. For example at 500-MeV IPNS has an effective flux approximately 10 times greater than the hot source at the Institute Laue Langevin (Grenoble, France).

The instruments for elastic or total scattering consist of two powder diffractometers (one a general purpose diffractometer and one a special environment diffractometer) which have excelled at high-resolution work and have also proven useful for studying amorphous systems. A single-crystal diffractometer is based on the Laue technique with a position-sensitive two-dimensional (30×30 cm) detector. A small-angle diffractometer also includes a position-sensitive detector, and is used for both metallurgical and biological problems. Of particular interest is the possibility of using epithermal neutrons in resonance small-angle scattering on biological molecules.

For inelastic scattering the crystal-analyzer spectrometer is particularly well suited to examine dispersionless high-energy vibrational modes. Two chopper spectrometers have proved exceptionally versatile in a variety of problems involving measurements of inelastic cross sections.

A new instrument, an electron-volt spectrometer, is under construction.

In the first year of operation approximately 120 experiments were performed at IPNS in the 3370 h of research time that was available. People from 23 universities, 5 industrial laboratories, 5 U. S. National Laboratories, and 8 foreign institutions were involved.

For additional information contact T. G. Worlton, Scientific Secretary, IPNS, Argonne National Laboratory, Argonne, IL 60349.

G. Weapons Neutron Research/Proton Storage Rings (WNR/PSR) Facility, Los Alamos, NM

The WNR is already operational as a high-intensity spallation neutron source. The user program was scheduled to begin in September 1983. Two-thirds of the neutron scattering beam time will be allocated for outside use and one-third reserved for in-house use. The first two user instruments will be the Be–BeO filter difference spectrometer (especially suited for chemical spectroscopy, and for studies of density of vibrational states and of optical modes of solids), and the single-crystal diffractometer (wavelength-resolved Laue camera). New instruments will be added to the user program as they become available and reach maturity. The tentative list of WNR instruments with their year of first operation and projected year for entry into the user program is: (1) filter-difference spectrometer (1980, 1983); (2) single-crystal diffractometer (1980, 1983); (3) liquids, amorphous, and special environment diffractometer (1980, 1984); (4) powder diffractometer (1980, 1984); (5) constant wave-vector-change spectrometer (1983,1985); (6) electron-volt spectrometer (1980,1985); (7) chopper spectrometer (1984,1986); and (8) small-angle diffractometer (1986,1987).

Some highlights of the research program to date include: (1) model-independent determination of the hydrogen–hydrogen pair correlation function in liquid water; (2) determination of the structure of the first molecular hydrogen complex; (3) observation of a new correlation of hydrogen bond vibrational frequencies with bond length for very short hydrogen bond; (4) development of the nuclear-resonance filter-difference method for electron-volt spectroscopy; and (5) observation of hydrogen momentum distributions in hydrides and water by scattering in the impulse approximation.

For additional information contact R. N. Silver, Group P-S, MS-H805, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545.

II. SYNCHROTRON RADIATION SOURCES

The five synchrotron radiation sources in the United States are described here. The newest entrant in the field, the NSLS, is still in the process of coming into full-scale operation, and the others are still undergoing enlargement and improvement. This is a rapidly growing area of research throughout the industrialized world.

Figure 1 is an aerial view of the Stanford Synchrotron Radiation Laboratory.

FIG. 1. An aerial view of the Stanford Synchrotron Radiation Laboratory.

A. Standford Synchrotron Research Laboratory (SSRL), Palo Alto, CA

SSRL is a national facility for the utilization of synchrotron radiation in biology, physics, materials science, medical science, and other disciplines. It is funded by the Department of Energy. The radiation comes from the storage ring, SPEAR, a facility within the Stanford Linear Accelerator (SLAC) built originally for high-energy physics research.

SPEAR is dedicated to the production of synchrotron radiation half of its operating time. During this time high currents of electrons, up to 100 mA are stored at high energies (3–3.5 GeV). The other half of the time the ring operates for high-energy physics research purposes to produce colliding beams of electrons and positrons. The ring is in operation between 8 and 9 months out of each year.

In addition to scientific research the Laboratory had a commitment to the development of advanced insertion devices for the enhancement of synchrotron radiation and the development of state-of-the-art instrumentation for the utilization of synchrotron radiation.

At present SSRL has 16 experimental stations on five beam lines covering the spectrum from 6 to 40 000 eV. A wide variety of experimental equipment is available for the user, and there are no charges either for the use of the beam or of the facility-owned support equipment. Both a 54-pole wiggler line and an undulator beam line serving three experimental stations are being developed; they will cover a range from 10 to 1000 eV.

SSRL is currently used by approximately 550 scientists from 124 different institutions, including universities, private corporations, and government laboratories.

As of March 1983 a total of 797 proposals had been received since March 1974, out of which 190 were active. A typical project involves four to eight scientists, including graduate students and post doctorals. Approximately 100 graduate students from 15 different universities work at SSRL each year. Over 200 publications based on research conducted at SSRL appear in journals each year.

For additional information contact A. Bienenstock, Director, Stanford Synchrotron Radiation Laboratory, P. O. Box 4349, Bin 69, Standford, CA 94305.

B. Cornell High Energy Synchrotron Source (CHESS), Cornell University, Ithaca, NY

CHESS, the Cornell High Energy Synchrotron Source, is a national laboratory which provides six x-ray experimental stations. X rays come from an 8-GeV electron storage ring (CESR). Monochromatic tunable photon beams from 4 to 100 keV are available. A six-pole 1.8-T wiggler provides a particularly intense spectrum with a critical energy in excess of 30 keV. The CHESS x-ray spectrum has a unique time structure—pulses come at 2.56 μs intervals with a pulse width of 0.13 ns.

Two stations provide white-beam capabilities, particularly useful for topography, high-pressure studies, and experiments that contain their own unique monochromators. A four-axis Huber diffractometer and two Picker diffractometers are available for diffraction physics experiments. Two complete EXAFS stations with data-acquisition software and off-line analysis packages are provided.

CHESS is supported by the National Science Foundation and currently provides experimental capabilities for approximately 100 active research proposals from all over the U. S. A.

For additional information contact Nancy Miller, Pro-

posal Administrator at CHESS, Wilson Laboratory, Cornell University, Ithaca, NY 14853.

C. National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY

The National Synchrotron Light Source (NSLS) is designed to provide the world's brightest continuous source of x rays and UV radiation. It is also the first x-ray facility in the United States dedicated for use as a synchrotron light source. It consists of two electron storage rings, one at 750 MeV for the production of vacuum ultraviolet (VUV) radiation, and one at 2.5 GeV for the production of x rays. In mid-1983 the VUV storage ring was in reliable operation with currents up to 300 mA and a lifetime of 2 h at 100 mA. The x-ray ring had stored beam, and initial operation for experimenters was expected during the latter part of 1983.

The VUV ring has 16 ports for VUV and IR research. It incorporates a unique free-electron laser designed to be a narrowband (relative bandwidth of 10^{-5}), continuously tunable (2000–4000 Å) UV source with average power in the range from one to several watts. The free-electron laser undulator can be used during routine storage ring operations to produce intense radiation between 100 and 2000 Å. The x-ray storage ring has 28 ports. Each of the 16 VUV and 28 x-ray ports is divided into two or three individual beam lines.

Under construction are several wiggler and undulator magnets which will significantly increase the photon energy and brightness.

The facility has a wide range of research equipment for basic and applied studies in condensed matter, surface science, photochemistry and photophysics, lithography, crystallography, small-angle scattering, metallurgy, x-ray microscopy, etc.

The NSLS is a national user facility, available without charge to university, industrial, national laboratory, and government users. There are several modes of use of the experimental facilities. A large number of beam lines have been designed and constructed by 27 participating research teams (PRTs). The PRTs are, for most part, user groups from outside Brookhaven National Laboratory with large, long-range programs which have been approved by the NSLS Program Advisory Committee. The PRTs are given priority for up to 75% of the operational time of their beam lines. General users will be scheduled for both PRT beam lines and for lines built by NSLS for the community in general.

For additional information contact M. Blume, Chairman, National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY 11973.

D. Synchrotron Radiation Center, University of Wisconsin, Stoughton, WI

The Synchrotron Radiation Center (SRC) of the University of Wisconsin operates the Tantalus 240-MeV electron storage ring and is bringing on line the Aladdin 1-GeV ring. When Aladdin is in operation, it will have 35 equivalent bending magnet source points and one inverse Compton scattering source point. Ten beam lines will be fully instrumented and maintained by the SRC. Monochromators will span the spectral range from about 4 to 1200 eV; there are plans to develop a soft x-ray crystal monochromator to extend the range to 4000 eV. Beam lines and monochromators will be available to users on a request-for-time basis. Since no single monochromator is able to span the entire range made available by Aladdin, requests for beam time should be specific on the choice of monochromator or the spectral range needed.

In addition to the ten facility beam lines, thirteen beam lines are being implemented by groups of users, called participating research teams (PRTs), each with its own specific purpose. Access to these instruments will be possible through negotiations involving the SRC director and the PRT involved.

When completed, Aladdin will have 23 monochromators operating on 21 beam lines, including five high-flux Seya-Namioka's (5–50 eV), three normal-incidence monochromators (including a 4-m ultrahigh resolution instrument), five toroidal grating monochromators (6–180, 225, and 700 eV), three high-resolution grasshoppers (20–1,000 eV), five high-resolution extended range grasshoppers (5–1500 eV), and a soft x-ray emission spectrograph. In addition, one x-ray crystal/grating (800–4000 eV) instrument has been authorized and a second is proposed.

Special facilities planned include an inverse Compton scattering line; a facility to handle transuranic, radioactive materials; soft x-ray lithography; ultraviolet and soft x-ray photoelectron spectroscopy systems with angle-integrated and angle-resolving capabilities; circular and magnetic circular dichroism; reflectance and absorption spectroscopies; and photon stimulated desorption.

Aladdin will operate—and Tantalus does operate—as a dedicated synchrotron source on a five day per week schedule with 48.5 h of beam time available for research. As with other national facilities, the user is responsible for the operation and the safety of his own instrumenation. The operation of the laboratory facilities is overseen by the SRC staff. The Physical Sciences Laboratory (PSL) of the University of Wisconsin provides the necessary support for the users, including computer capabilities (a VAX 11/780), purchasing services, mechanical and electrical engineering services, an outstanding machine shop, a library, and a stockroom. Housing is available at the PSL Guest House.

For additional information contact E. M. Rowe, Director, Synchrotron Radiation Center, 3725 Schneider Drive, Route 4, Stoughton, WI 53589.

E. NBS Synchrotron Radiation Facility, National Bureau of Standards, Gaithersburg, MD

The Synchrotron Ultraviolet Radiation Facility (SURF-II) at the National Bureau of Standards is a 280-MeV electron storage ring used as a dedicated light source in two areas of science: radiometry and experimental physics. Since the facilities for each of these two uses are for the most part independent, they are described separately.

The radiometric facilities fall into two classes: calibration and radiometric standards. SURF-II is an ideal light source for calibration since it is a single-magnet accelerator

with a perfectly circular orbit. This feature allows the spectral distribution from the ring to be calculated with an accuracy of 2%. The calibration beam line consists of a white light port with accurate baffling to ensure a well-defined light beam. The beam light is equipped with a two-axis, two-transition gimbal on which a vacuum chamber or windowed instrument can be mounted. After an instrument is mounted, it is rotated about its entrance slit so that the light beam is scanned over its entire optical surface. For instruments which do not have their own vacuum envelope, e.g., rocket-borne or space-shuttle spectrometers, the beam line can be attached to a large vacuum chamber (4×4×8 ft) capable of attaining 10^{-8} Torr. A two-axis goniometer in the chamber again allows the mounted instrument to be rotated and the entire optical surface to be calibrated.

The radiometric standards beam line is used primarily for the calibration of photodiodes which are sold by NBS. It consists of a toroidal grating monochromator to disperse the light, a double ionization chamber to measure absolute photon intensity, and the diode chamber. Each diode is calibrated as a function of photon energy and is available as a secondary photometric standard. The calibration covers the photon energy range from 5 to 100 eV.

The facilities for experimental physics consist of three beam lines equipped with four monochromators. The first instrument is a high-flux, normal-incidence monochromator equipped with a differential pumping chamber to allow windowless gas-phase experiments. A pressure of 10^{-4} Torr can be maintained in the experimental chamber while the ring is operating. The spectral range is from 350 to 2000 Å, with a resolution of 0.05 Å. The maximum intensity is 10^{11} photons per second out of the exit slit.

The second instrument is a grazing-incidence, Rowland circle monochromator with an experimental chamber designed for reflectivity measurements. It covers the range from 80 to 800 Å, with a resolution of 0.15 Å. A gimbal in the experimental chamber allows a channeltron electron multiplier detector to be scanned about the sample.

The third monochromator has a range of 165 to 500 Å, with a resolution of 1 Å and an output of 10^9 photons per second on the sample in a 2-mm-diam spot. A reentrant arrangement allows the sample to be placed within 2 cm of the slit. The experimental chamber contains a cylindrical mirror analyzer for surface-science studies. Both electron and ion emission from well-characterized surfaces can be studied.

The fourth monochromator is similar to the third one, but with a spectral range from 300 to 1000 Å. There is no permanent experimental chamber attached to it.

All these instruments are equipped with dedicated computers for experimental control and data acquisition.

Several monochromators are under construction. One is for a new radiometry facility which will also be available for experimentation. The second is a new high-flux, ultra-high-vacuum monochromator to replace the surface-science facility. This instrument was being installed during the fall of 1983. Finally, a normal incidence monochromator with a resolving power of 10^5 is scheduled to be in operation by the summer of 1984.

For additional information contact R. P. Madden, or D. L. Ederer, National Bureau of Standards, Washington, DC 20234.

III. FACILITIES FOR MICROANALYSIS, MICROFABRICATION, AND SURFACE STUDIES

The five facilities described in this section provide a great variety of sophisticated devices for probing, characterizing, and altering the structures of materials, and for preparing new materials and new structures. Surfaces and microstructures command a large share of the effort. It is worth noting that these facilities allow numerous powerful techniques to be brought to bear simultaneously on a single problem.

Figure 2 shows a small section of an array of resonant elements—dipole openings in a gold film deposited on calcium fluoride—fabricated at NRRFSS (see Sec. A below). The array acts as a band rejection transmission filter in the mid-infrared (7–9 μ). The primary resonant frequency is one-hundred times higher than any previously reported.

A. National Research and Resource Facility for Submicron Structures, Cornell University, Ithaca, NY

In 1977 the National Science Foundation established a National Research and Resource Facility for Submicron Structure (NRRFSS) to help advance submicron science and technology. The specific objectives of NRRFSS are: (1) to promote and carry out research to advance the art of submicron fabrication technology, and to train scientists and engineers in this field; (2) to provide a resource primarily for use by the university community to fabricate advanced devices or research structures which require submicron dimensions; (3) to stimulate innovative research outside the electrical engineering device community which will shed light on fundamental physics or materials problems limiting submicron technology; and (4) to keep the technical community informed on progress at the Facility.

Microfabrication research at NRRFSS involves about one hundred Cornell graduate students representing about eight departments and thirty-five faculty members. In addi-

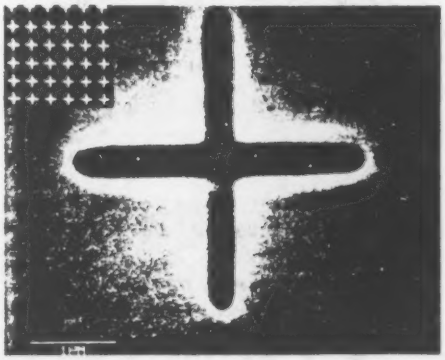

FIG. 2. A small section of an array of resonant elements fabricated at NRRFSS. Enlargements of one element, 3 μ long, also shown.

tion there are currently about thirty approved user projects outside Cornell. The Cornell research includes both facility development research and user research. The facility development research emphasizes enhancement of equipment and techniques in advanced lithography and dry pattern transfer processing as well as thin-film growth, deposition, and modification and, to a lesser extent, advanced device technologies and thin-film electrical, chemical, and structural analysis. Both facility development research and user research projects are initiated by a proposal review process.

For additional information contact E. D. Wolf or R. A. Brown, NRRFSS, Knight Laboratory, Cornell University, Ithaca, NY 14853.

B. The Center for Microanalysis of Materials, University of Illinois, Urbana, IL

It is not possible for an individual group to support equipment and maintain an interest in all of the techniques of microanalysis. The result is that, in general, a research group specializes in a particular characterization technique and tailors its research to it. The University of Illinois has adopted a different approach: instrumentation for microcharacterization of materials has been gathered into the Center for Microanalysis of Materials that operates as a facility for all of the materials research programs on campus and many collaborative research programs with other universities and laboratories.

The Center has transmission electron microscopes, scanning electron microscopes, a scanning transmission electron microscope, electron microprobes, scanning Auger microscopes, secondary ion microprobes, an x-ray photoelectron spectroscopy unit, rotating and fixed anode x-ray sources fitted with instrumentation for EXAFS, topography, small-angle scattering and all standard x-ray methods, and an accelerator for backscattering spectroscopies. Most of these instruments are modern commercial machines fitted with a wide range of accessories and instrumentation. In addition the Center has extensive facilities for specimen preparation. The Center is operated by a staff of about a dozen professionals/academics who guide and collaborate in research, maintain the equipment, and give instruction for its use.

More than a hundred faculty members on the University of Illinois campus carry out research in materials science. The Center for Microanalysis of Materials provides them with the unique opportunity to use almost any microanalytical technique, or combination of techniques, to characterize their samples.

A flexible program of interaction with other institutions is also maintained. For additional information contact J. A. Eades, Materials Research Laboratory, University of Illinois, 104 S. Goodwin, Urbana IL, 61801.

C. ORNL Surface Modification and Characterization Collaborative Research Center, Oak Ridge, TN

The Oak Ridge National Laboratory Surface Modification and Characterization Collaborative Research Center (SMAC) is a facility for cooperative research involving university and industrial scientists working with ORNL personnel on problems of mutual interest. The goal of the center is to provide and maintain advanced processing and characterization techniques for *in situ* alteration and analysis of near-surface properties of a wide range of materials.

The materials processing capabilities of the Center feature ion implantation doping, ion beam and laser mixing, and pulsed-laser processing. These are all nonequilibrium processing techniques capable of achieving new and often unique materials alterations not possible with equilibrium processing methods. The *in situ* materials characterization capabilities emphasize ion scattering and nuclear reaction analysis, ion channeling, surface analysis techniques (LEED, Auger, etc.), and other property measurements such as electrical resistivity and optical reflectivity.

The SMAC facility is equipped with beam lines from positive-ion analysis accelerators and a high-current ion implantation accelerator integrated into common ultra-high-vacuum chambers (10^{-10} Torr) which contain surface analysis instruments, solid-state detectors, and UHV goniometers and sample holders, as well as optical windows which allow *in situ* laser processing. With these facilities it is possible to alter materials properties in UHV by ion beam and laser processing at sample temperatures from 4 to 1,300 K, and to analyze the materials in place. The ion accelerators include a 2.5-MeV Van de Graaf, a 200-keV high-current implantation accelerator, and a 1.7-MeV tandem accelerator, with both duoplasmatron and heavy-ion sources. The latter is scheduled for operation in 1984. A wide range of high-powered lasers is available, including ruby, Nd:Yag, and KrF lasers (15×10^{-9} s pulse duration time); a mode-locked Nd:Yag laser (30×10^{-12} s pulse duration time); and a cw Ar ion laser. With these laser sources it is possible to achieve heating and cooling rates that vary from approximately 10^6 to approximately 10^{12} °C per second in the near-surface region.

Facilities in the Center are being expanded to accommodate more users. For additional information contact B. R. Appleton, Solid State Division, ORNL, Oak Ridge, TN 37830.

D. SHaRE Program, Oak Ridge National Laboratory, Oak Ridge, TN

The SHaRE Program is a collaborative research venture in materials science between the research staff of ORNL and the research staff at both universities and industrial laboratories. Managed by Oak Ridge Associated Universities, its purpose is twofold: (1) to permit ORNL research staff members to carry out additional research relevant to the Department of Energy programs that would not ordinarily be possible; and (2) to make available to university staff and industrial researchers sophisticated research equipment at ORNL which is not available in their home institutions.

All research sponsored at ORNL under the SHaRE program is collaborative, with at least one ORNL staff member and one senior researcher from the outside institution having joint responsibility for successful completion of each project and for publication of the work.

From its inception in late 1978, the SHaRE program has concentrated on the application of advanced microanalytical techniques to research areas in materials science. Centered in the Metals and Ceramics Division, the facilities used under the SHaRE program include the analytical electron microscopes, the high-voltage electron microscope facility, the Auger electron spectrometry/surface microanalytical apparatus, the Van de Graaf nuclear backscattering equipment, and the computer facilities. Once a project is established as a collaborative SHaRE program, there is no charge for the use of the facilities. Access to the program requires submission of a proposal which involves an interested ONRL collaborator.

For additional information contact E. A. Kenik, Metals and Ceramics Division, Oak Ridge National Laboratory, P. O. Box X, Oak Ridge, TN 37830.

E. Regional Instrumentation Facility (CRISS), Montana State University, Bozeman, MT

The regional Instrumentation Facility at the Montana State University Physics Department (CRISS: Center for Research in Surface Science and Submicron Analysis) is devoted principally to basic and applied research in surface physics and chemistry. The main instrumentation includes: (1) a scanning Auger microprobe; (2) a high-resolution electron-energy-loss spectrometer with double-pass monochromator and analyzer; and (3) an ESCA system with Al/Mg double-anode x-ray head and hemispherical analyzer; the ESCA system is housed in the same vacuum as (2).

A singular advantage of this arrangement is the possibility of doing ELS and ESCA experiments in conjunction. The ESCA analyzer can do ion scattering spectroscopy in conjunction with the ion gun. The chamber supports a SIMS add-on based on a quadrupole mass analyzer. A third vacuum chamber supports a low-resolution (5-μ beam size) scanning Auger spectrometer and a He-discharge lamp for Ultraviolet Photoemission Spectroscopy. The laboratory also has the usual support facilities.

Although the advice and assistance of the staff are available to whatever extent necessary for effective execution of the experiments, the laboratory is operated primarily as a user facility, and the users are expected to plan and execute their own experiments, devoting the necessary time (from 1 to 3 days) to learn the operation of the equipment. The user's stay at the facility is generally from one to three weeks.

The staff includes a director, two staff scientists, a technician, and an administrative assistant. For additional information contact G. J. Lapeyre, Physics Department, Montana State University, Bozeman, MT 59717.

IV. ELECTRON MICROSCOPES

High voltage and ultrahigh resolution in electron microscopy require large installations. The three installations described here provide advanced capabilities for users. An example of the work is shown in Fig. 3, which is a micro-

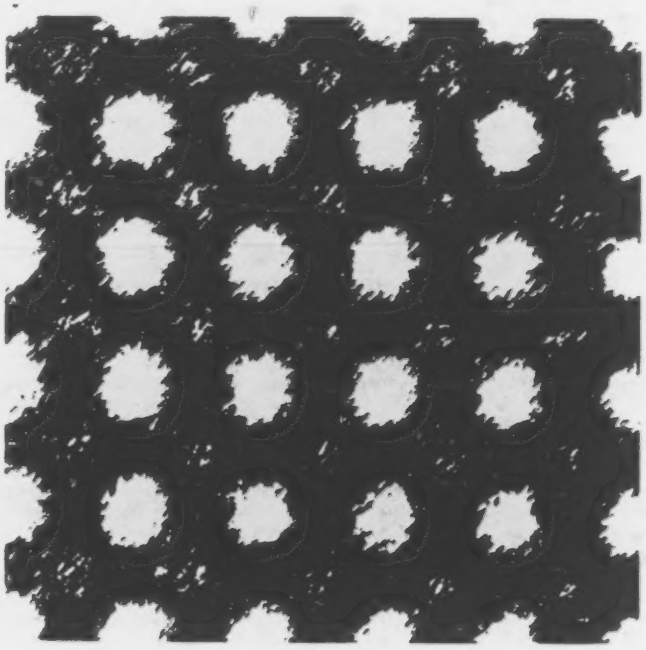

FIG. 3. Micrograph of zirconium dioxide with atomic resolution, taken on the JEM ARM-1000 at the National Center for Electron Microscopy.

graph of zirconium dioxide with atomic resolution. All atomic positions in a (0 0 1) projection are shown. The photograph was taken on the JEM ARM-1000 at the National Center for Electron Microscopy.

A. Facility for High Resolution Microscopy, Arizona State University, Tempe, AZ

The Facility for High Resolution Microscopy in the Center for Solid State Science at the Arizona State University is supported by the National Science Foundation and the State of Arizona. The goals of the Facility are to advance the methods and instrumentation of electron microscopy; to apply new research methods to the structural analysis of solids, particularly in the areas of materials science, solid-state physics, solid state chemistry, and geology; and to provide high-resolution research facilities for use of scientists and engineers from the solid-state science community at large. In addition, the Facility conducts topical research conferences and advanced electron microscopy schools each January.

The principal research topics of current interest are high-resolution imaging of surfaces and interfaces, electron-loss spectroscopy, microdiffraction, and energy dispersive x-ray spectroscopy. There are, at present, six electron microscopes at the facility, including two field-emission-source instruments (EM400/ST and HB-5) and a fixed-beam imaging instrument with 2.5-Å resolution. The field-emission-source instruments have been shown capable of high coherent microdiffraction from specimen areas as small as 5 Å, and microspectroscopy from areas about 10 Å in diameter. These experimental methods are being applied to an increasing number of intriguing problems, particularly in the areas of electronic materials, surfaces, and catalysts.

During the last year, more than twenty outside scientists conducted research at the Center with the assistance of an on-site support staff, and about forty on-site research programs made use of the Facility.

The topic of the January 1983 Research Conference at the Facility was High Resolution Imaging and Microanalysis of Surfaces. The conference topic for January 1984 is High Resolution Structural and Chemical Analysis of Boundaries and Interfaces.

For additional information contact the Director, Facility for High Resolution Electron Microscopy, Center for Solid State Science, Arizona State University, Tempe, AZ 85287.

B. National Center for Electron Microscopy, Lawrence Berkeley Laboratory, Berkeley, CA

The National Center for Electron Microscopy (NCEM) is primarily a high-voltage electron microscope facility with instrumentation designed for ultrahigh resolution or dynamic *in situ* imaging of materials. The Center is supported by the U. S. Department of Energy, and its instruments have been designated as user facilities.

Among the unique microscopes in the NCEM is a Kratos EM-1500, the only instrument in the U. S. which provides accelerating voltages in the 1200–1500-kV range. It features both a top-entry goniometer stage for high-resolution work and a side-entry stage for dynamic *in situ* and environmental cell studies. Depending upon the choice of specimen holder, the sample can be viewed over a plus or minus 45 deg tilt angle, at temperatures ranging from ambient to 850 °C and with various gaseous environments up to 1 atm pressure. Dynamic events can also be recorded on video tape. The operating pressure in the optical column can be brought to 10^{-7} Torr and the microscope has demonstrated a point-to-point resolution of about 3 Å.

A second instrument is the JEM ARM-1000, the only instrument of its kind in the world, providing a point-to-point resolution of 1.7 Å or better over all operating voltages up to 1000 kV. It has a top-entry goniometer stage with 45 deg biaxial tilting and height adjustment which, in addition to variable focal length, enables convergent beam electron diffraction patterns to be taken from the same specimen areas imaged in high resolution. Operating pressures are in the 10^{-8}-Torr range. The microscope makes extensive use of microprocessor control for precise operation, and has very high brightness (10^{9} A/cm^2 ster) due to its lanthanum hexaboride filament design.

Other microscopes within the NCEM include a JEOL JEM 200CK with an ultra-high-resolution goniometer and a Hitachi HU-650 high-voltage electron microscope with hot stage and environmental cell. By September 1983 a new building addition should have been completed to house the remainder of the NCEM support equipment, including wet and dry specimen preparation laboratories, optical diffractometer, image analysis and processing hardware, and an on-site minicomputer-based image simulation laboratory to assist with micrograph interpretation.

Beam time of the NCEM microscopes is allocated after review and acceptance of research proposals submitted in advance. In accordance with Department of Energy policy, as long as the proposed work is of documented programmatic interest to the Department and the results are published in the open literature, there is no charge for use of the NCEM microscopes.

For additional information contact G. Thomas, Scientific Division, or K. H. Westmacott, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, Berkeley, CA 94720.

C. HVEM-Tandem-Accelerator National User Facility at Argonne National Laboratory, Argonne, IL

The High Voltage Electron Microscope (HVEM)-Tandem Facility is a unique national research facility. It is supported by the U. S. Department of Energy and is available to scientists from industry, universities, and other national laboratories, after approval of submitted research proposals The facility is operated by the Materials Science and Technology Division of ANL and provides a unique combination of capabilities for high-voltage electron microscopy, ion implantation/bombardment, and ion beam analysis. A number of side-entry stages permits *in situ* experiments in the temperature range from 10 to 1300 K *in vacuo*, and from ambient to 1300 K in noncorrosive gaseous atmospheres. Straining stages are available for deformation and fracture studies over a wide range of experimental conditions. The

HVEM/ion beam interface permits direct observation of the effects of electron and ion bombardment on materials in the microscope. The ion beam interface may be used with either a 300-kV ion accelerator or the 2-MV tandem ion accelerator. Calibrated dosimetry systems are available for both ion and electron beams.

Prime-time usage of the facility is divided approximately equally between ANL and non-ANL scientists. The facility staff is available during one or two shifts a day to instruct experimenters in the use of the equipment, and in some intances to participate in experimental programs. In general researchers are expected to become competent to operate the equipment. A course of lectures on high-voltage microscopy supplemented by lecture notes is available on video tape.

When not scheduled for use with the HVEM the 2-MV Tandem and the 300-kV accelerators are used separately from the microscope by the ANL staff. Outside users wishing to use the accelerators alone are requested to collaborate with the appropriate group of the Materials Science and Technology Division of ANL.

For additional information contact the Facility Secretary, Sheryl Ruffatto, Building 212, Argonne National Laboratory, Argonne, IL 60439.

V. OTHER FACILITIES

This section lists several facilities that do not fit in the foregoing categories. They are the Francis Bitter National Magnet Laboratory, which provides ultrahigh magnetic fields of various kinds; the Los Alamos Equation of State Library, which provides the latest information on matter under extremes of pressure and temperature; and the Combustion Research Facility, which provides powerful new capabilities for the study of combustion in engines and other systems.

A. The Francis Bitter National Magnet Laboratory, M.I.T., Cambridge, MA

The Francis Bitter National Magnet Laboratory is the largest facility in the world for generation of intense continuous magnetic fields. The Laboratory traces its origin to the work of Prof. Francis Bitter, who pioneered electromagnetic technology in the 1930's; it was organized as a national laboratory in 1960 and started its operation at the present site in 1963. The National Science Foundation has been sponsoring the Laboratory's operation since 1970.

The Magnet Laboratory's facilities are available to users free of charge. A variety of high-field magnets are provided, together with cryogenic measurement and data processing equipment. Experienced support staff is also available on a full-time basis to assist visitors with all aspects of their experiments. Research staff at the Laboratory can be consulted about problems in specialized areas.

The Laboratory features almost two dozen water-cooled (Bitter) magnets in five bore diameters from 3.3 to 24.8 cm, with fields as high as 25 T in a 5.4-cm bore and 30 T in a 3.3-cm bore.

All fields are calibrated to 0.1% and are repeatable and stable to 0.05% short term, and 0.1% long term. Time stability of a few parts in 100 000 can be obtained with a localized feedback system. This system makes it possible, for example, to do nuclear-magnetic-resonance experiments in spatially uniform fields and to reduce eddy-current heating in low-temperature experiments. At the other extreme, modulation fields of up to 0.5 T peak-to-peak at 7.5 Hz can be generated for use with ac signal processing in, for example, quantum oscillatory experiments. The dc fields can be swept continuously from zero to maximum in as little as 1 min or as much as 2 h. Field setting, sweep, and modulation are all under local control by the user.

Two new sets of magnets should become available soon: (1) a pulsed-field facility which offers fields up to 45 T with 10-ms duration in a 1-cm bore at 4.2 K (1.5-cm bore at 77 K); (2) a superconducting magnet with a 20-min sweep to a 15-T field and a 5-cm room temperature access.

Users have available to them a broad range of equipment and apparatus, including complete temperature control systems with a range from 1.5 to 300 K, helium-3 and dilution refrigerators, and a complete de Haas—van Alphen apparatus along with homogeneous fields up to 24 T.

There is a queue of approximately three months for reserved magnet time—which is assigned in blocks of 15 to 30 h, depending on the power required. First-time users, however, can usually be accommodated within several weeks, and all users have the option of requesting magnet time on a recurring, biweekly basis. There is a separate queue for the use of the hybrid magnets.

For additional information contact Larry Rubin, Francis Bitter National Magnet Laboratory, NW-1108, M. I. T., Cambridge, MA 02139.

B. The Los Alamos Equation-of-State Library (SESAME), Los Alamos National Laboratory, Los Alamos, NM

The SESAME Equation-of-State (EOS) Library is a standardized, computer-based library of tables of thermodynamic properties and FORTRAN subroutines developed and maintained by the Equation-of-State and Opacity Group of the Theoretical Division of Los Alamos National Laboratory.

The Library contains data for about 70 materials, including metals, minerals, polymers, mixtures, etc., as well as simpler atomic and molecular species. The Library is being offered to all interested users free of charge.

The thermodynamic data stored in the Library include tables of pressure P and energy E (and also, in some cases, of Helmholtz free energy A), each as a function of density and temperature. Besides total P, E, and A tables, in many cases separate tables of thermal, electronic, and ionic (including zero point) contributions to P, E, and A are available. The SESAME EOS Library also has opacity data with a low-temperature limit of about 1 eV.

For further information on the SESAME EOS Library, write to SESAME Library, T-4, MS B925, Los Alamos National Laboratory, Los Alamos, NM 87545. Users interested in the opacity data should contact A. L. Merts or M. F. Argo, T-4, MS B212, Los Alamos National Laboratory, Los Alamos, NM 87545.

C. Combustion Research Facility, Sandia National Laboratories, Livermore, CA

The Combustion Research Facility (CRF) at Sandia National Laboratories in Livermore provides scientists an opportunity to study all phases of combustion science and technology. Researchers from universities, industry, and other government laboratories are encouraged to use the many laboratory and computer facilities, and to collaborate with resident scientists studying the basic chemistry and fluid mechanics of flames, as well as combustion phenomena occurring in devices such an engines and coal combustors. Central to nearly all CRF research is the incorporation of the most advanced laser-based techniques, many of which are being developed at the facility.

One part of this program is supported by the Division of Materials Sciences, Office of Basic Energy Sciences, U. S. Department of Energy, to develop a better understanding of the degradation of ceramic coatings and metallic alloys in the hot, corrosive, particulate-laden environments often present in combustion systems. Here, too, the application of the latest optical techniques has been strongly emphasized. Examples of such techniques, which are either in development or in use to study relevant problems, are:

(1) *In situ* surface Raman spectroscopy, which provides nonintrusive, real-time measurements of the chemical compositions and structural phases of corrosion layers building up on the surfaces of exposed materials.

(2) Raman microscopy, wherein Raman spectra are obtained with 1-μ resolution for the detailed characterization of polycrystalline or amorphous materials typical of most corrosion layers.

(3) Sputter-induced photon spectroscopy, in which optical emissions from excited atoms sputtered from surfaces provide high sensitivity for detecting trace species, including hydrogen, in insulating as well as conducting materials.

(4) Sputter-Raman spectroscopy, in which Raman spectroscopy is used to determine the depth profile of corrosion layers as material is removed by sputtering.

For additional information contact Walter Bauer, Department 8340, Sandia National Laboratories, Livermore, CA 94550.

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APPENDIX B

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APPENDIX C

PRESENTATIONS TO THE MAJOR MATERIALS FACILITIES COMMITTEE

CONTENTS

FOREWORD

I. WORKSHOP: MARCH 17-19, 1984*

A. INTRODUCTION

Probing Matter with Electrons, Neutrons, and Photons
J. D. Litster, Massachusetts Institute of Technology

B. SCIENTIFIC OPPORTUNITIES WITH SYNCHROTRON RADIATION
D. W. Lynch, Iowa State University, Chairman

1. X-Ray Physics
D. E. Moncton, Brookhaven National Laboratory
2. Scientific Opportunities with Vacuum Ultraviolet (Soft X-Ray) Synchrotron Radiation from Insertion Devices
J. Stohr, Exxon Research & Engineering Company
3. X-Ray Microprobe Characterization of Materials: The Case for Undulators on Advanced Storage Rings
C. J. Sparks, Jr., Oak Ridge National Laboratory
4. Synchrotron Radiation Research in Biology and Medicine
K. Hodgson, Stanford University

C. SCIENTIFIC OPPORTUNITIES WITH NEUTRONS
R. J. Birgeneau, Massachusetts Institute of Technology, Chairman

1. Physics
J. D. Axe, Brookhaven National Laboratory
2. Chemistry
B. Fender, Institut Laue-Langevin

* S. A. Rice, University of Chicago, and J. D. Litster, Massachusetts Institute of Technology, served as Co-Chairmen of a panel discussion on March 17.

3. Scientific Opportunities with Neutrons in Materials Science
   J. R. Weertman, Northwestern University
4. Application of Neutron Beam Research in Biology and Medicine
   P. B. Moore, Yale University

D. OVERVIEW OF RELATED REPORTS

1. Current Status of Neutron Scattering Research and Facilities the United States
   S. A. Werner, University of Missouri
2. Planning Study for Advanced National Synchrotron Radiation Facilities
   M. L. Knotek, Sandia National Laboratories

E. PROPOSED NEW AND UPGRADED FACILITIES FOR SYNCHROTRON RADIATION RESEARCH
   D. W. Lynch, Iowa State University, Chairman

1. Prospectus for a 6 GeV Synchrotron Source, Argonne National Laboratory
   Presented by K. L. Kliewer
2. Planned Evolution of the NSLS, Brookhaven National Laboratory
   Presented by D. E. Moncton
3. A Prospectus for a 6 GeV Dedicated Synchrotron Radiation Facility at Cornell University, Cornell High Energy Synchrotron Source
   Presented by B. D. McDaniel
4. The Advanced Light Source: Scientific Opportunities, Lawrence Berkeley Laboratory
   Presented by H. Grunder
5. SSRL's Planning for a New Synchrotron Radiation Facility including a 6 GeV Storage Ring, Stanford Synchrotron Radiation Laboratory
   Presented by A. I. Bienenstock and H. Wiedemann

F. PROPOSED NEW AND UPGRADED FACILITIES FOR NEUTRON SCATTERING
   R. J. Birgeneau, Massachusetts Institute of Technology, Chairman

1. The Argonne Neutron Plan, Argonne National Laboratory
   Presented by G. H. Lander
2. Guide Hall at the High Flux Beam Reactor, Brookhaven National Laboratory
   Presented by B. P. Schoenborn
3. WNR/PSR Experimental Hall Expansion, Los Alamos National Laboratory
   Presented by J. C. Browne

4. NBS Center for Cold Neutron Research, National Bureau of Standards
Presented by J. M. Rowe
5. ORNL Presentation to the Major Materials Facilities Committee of the National Research Council, Oak Ridge National Laboratory
Presented by R. M. Moon

G. THE ROLE OF NATIONAL LABORATORIES IN MATERIALS RESEARCH

1. The Role of National Laboratories in Materials Science Research
H. Postma, Oak Ridge National Laboratory
2. Synchrotron R&D at the Defense Programs Laboratories
P. E. Coyle, Lawrence Livermore National Laboratory
3. Overview of the Recent ERAB Report on Materials Research and Development
R. H. Pry, Gould, Inc.

II. COMMITTEE MEETING MAY 3, 1984

OTHER KINDS OF MAJOR MATERIALS FACILITIES
A. Narath, AT&T Bell Laboratories, Chairman

1. High Magnetic Field Research in the U.S. - Status of the National Facility and Future Opportunities
P. A. Wolff, Massachusetts Institute of Technology
2. The Materials Research Laboratory Program
W. D. Nix, Stanford University
3. Toward an Advanced Materials Processing and Analysis Center (AMPAC)
H. K. Bowen, R. M. Latanision, and J. B. Vander Sande, Massachusetts Institute of Technology

III. LIST OF RELEVANT REPORTS

IV. PARTICIPANTS AT THE WORKSHOP, COMMITTEE, AND PANEL MEETINGS

V. CORRESPONDENTS

APPENDIX D

PRESENTATIONS TO PANELS
OF THE MAJOR MATERIALS FACILITIES COMMITTEE

Neutron Scattering Panel
National Academy of Sciences, Washington, D.C.
February 26-27, 1984

Argonne National Laboratory: R. Kustom, G. Lander
Brookhaven National Laboratory: V. Emory, B. Schoenborn
Los Alamos National Laboratory: J. Browne, R. Silver
National Bureau of Standards: M. Rowe, C. Han
Oak Ridge National Laboratory: H. Mook, R. Moon, Jr.
Department of Energy Perspective: L. Ianniello
National Bureau of Standards Perspective: K. Kammer

Synchrotron Radiation Panel
Molecular Biology Institute
University of California at Los Angeles
February 28, 1984

A 1.6 GeV Storage Ring: D. Shirley, D.Attwood, Lawrence Berkeley Laboratory

A 6 GeV Storage Ring*: A. Bienenstock, H. Wiedemann, Stanford Synchrotron Radiation Laboratory; D. Mills, B. Battermann, Cornell High Energy Synchrotron Source; M. Blume, S. Krinsky, Brookhaven National Laboratory; K. Kliewer, Y. Cho, Argonne National Laboratory

* The speakers shared the time describing science for a 6 GeV machine; each devoted a modest fraction of his presentation to site-specific plans.

78

Other Specialized Facilities Panel
National Academy of Sciences, Washington, D.C.
March 8, 1984

UV Laser Sources: G. Rosenblatt, Los Alamos National Laboratory
National Magnet Laboratory: P. Wolff, Massachusetts Institute of Technology
Muon Sources: R. H. Heffner, Los Alamos National Laboratory

PUB-5101

REPORT OF THE

NCAM INDUSTRY PARTICIPATION WORKSHOP

May 23, 1983

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

This work was supported by the U.S. Department of Energy
under Contract DE-AC03-76SF00098.

Contents

Conclusions from the Workshop 1

List of Attendees 2

Summary of the Workshop Proceedings 6

Report from the Working Group on Industry Input on Programs 11

Report from the Working Group on Proprietary Constraints 15

Report from the Working Group on Technology and Personnel Transfer 16

Agenda 18

Conclusions from the Workshop

On May 23, 1983, research executives from fifteen high-technology companies attended a 1-day workshop at Lawrence Berkeley Laboratory to consider the problems and requirements for productive industry participation in NCAM. After hearing and discussing presentations on Lawrence Berkeley Laboratory, NCAM, technology transfer, and current DOE policies governing patents and work with or for industry, the attendees divided into three working groups. These groups considered respectively (1) industry input on programs, (2) proprietary constraints: the need to change existing regulations, and (3) technology and personnel transfer.

This workshop summary abstracts the introductory talks and the discussion, and it includes the reports submitted by each of the working groups. There were five major conclusions.

1) NCAM is a pioneering effort, well worth considerable effort and support, to produce a unique model in which industry, universities, and a national laboratory will work together for the benefit of the nation on research of interest to industry.
2) The nature and orientation of NCAM needs to be planned carefully to assure that it becomes part of the strategic thinking of industry.
3) The selection of research programs is critically important and should be done after consulting with industry and holding technical workshops. Three to five programs should be started initially.
4) DOE, Laboratory, and University policies on patents and data rights, publication delay, access by foreign nationals, assumption of liability, and protection of data will have to be modified to attract extensive industrial participation in NCAM.
5) Technology transfer can be accomplished most effectively through interchange of scientific personnel. Other means recommended are joint research projects, industry-funded projects and technical workshops.

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Mr. Mark Owens, Jr.
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Mr. Dennis Neely
Resident NCAM Representative

Summary of the Workshop Proceedings

The Workshop was opened by the Head of the Industry Participation Office, *Dr. Heinz Heinemann*, who welcomed the Industry Participants and explained that the morning would be spent in hearing and discussing presentations outlining NCAM's plans for industry participation and defining the type of advice sought. Workshop panels would discuss specific problems in the afternoon.

In his introductory remarks, he indicated the ways industry can participate in NCAM:

1) by providing members of the NCAM Policy Board,
2) by providing members of the Scientific Program Council,
3) by providing members of Laboratory Advisory Committees,
4) by exchanging scientific personnel, and
5) by utilizing graduate students and post-doctoral fellows trained at NCAM.

He outlined NCAM objectives:

1) Assemble interdisciplinary teams to tackle fundamental problems of broad significance in the area of materials research.
2) Obtain industrial advice on projects from inception to technology transfer.
3) Work in areas where costs and needed research tools restrict industry research.
4) Provide facilities where industry's scientific personnel may train and carry out research.
5) Educate a future generation of scientists in materials research areas.

He introduced the Laboratory Director, *Dr. David Shirley*. Dr. Shirley extended a welcome on behalf of Lawrence Berkeley Laboratory and gave the participants background on the Laboratory, its affiliation with the University of California, and its current structure and scientific strengths. Director Shirley observed that NCAM will be a major step in implementing U.S. Science Policy and that the center will provide support for U.S. energy-related and high-technology industries and increase strategic self-sufficiency through enhanced understanding of the synthesis, characterization, and properties of advanced materials.

Dr. Hermann Grunder, Associate Director of the Accelerator and Fusion Research Division, explained that the NCAM Program was being developed within the organizational structure of the LBL Accelerator and Fusion Research Division. He described the present national facilities at LBL, and the planned facilities for NCAM, including the Advanced Light Source.

Dr. Eugene Haller, NCAM Scientific Program Director, introduced the NCAM scientific program. He described the organizational structure of NCAM, showing the relationship of the

Advisory Committees to the LBL Director, NCAM Director and Laboratory Heads. He listed the four elements of NCAM: the Advanced Materials Synthesis Laboratory (AMSL), the Surface Science and Catalysis Laboratory (SSCL), the Advanced Device Concepts Laboratory (ADCL), and the Advanced Light Source, and he mentioned the research programs planned for each laboratory.

He stated that the objectives of NCAM were to

1) perform long term basic research of particular interest to industry and of importance to national needs,
2) gain the scientific knowledge required for the synthesis, the analysis, and processing of novel and advanced materials,
3) explore the synergistic relationship between novel materials and new devices,
4) advance the science of ideal and real surfaces, coatings, and interfaces,
5) provide graduate and post-graduate education for the next generation of engineer and scientists.

The Advanced Light Source was discussed in terms of its capabilities and how it would relate to NCAM research.

Dr. Heinz Heinemann stressed the need for industry input to assist NCAM in meeting its goals and reviewed some of the industry comments already received. In general these comments supported the proposed programs and recognized the need for greater government-industry collaboration in research. He also pointed out that there was considerable agreement in their suggestions of possible programs to be pursued.

Dr. J. William Morris, Jr., Deputy Head of the Industry Participation Office, described several possible forms of industry participation. Mechanisms include consultation in the design and identification of programs, joint support of research, collaborative research, provision for use of advanced facilities, participation in workshops, and interchange of scientific personnel. He mentioned advantages NCAM would offer industry, such as the utilization of advanced facilities, participation in collaborative research, and the provision of opportunities for education and training. He emphasized that NCAM's thrust would be in generic research, and that outgrowths of the program could include task-force research on specific topics, and follow-on research in industry laboratories.

Discussion followed Dr. Morris' presentation.
(Q = Question, A = Answer, O = Observation)

Q. Use of task forces to solve long-range generic problems has not been found to be very effective. What are your comments?

A. It is agreed that research goals must be well defined and a time schedule set. With these constraints, task forces can work productively on generic problems.

Q. Can NCAM work against set time schedules?

A. Yes, within limits.

Q. Antitrust regulations would appear to prohibit certain industries working in a task force with other industries (for example, Westinghouse and General Electric).

A. Perhaps collaborative efforts coordinated by a national laboratory would meet antitrust objectives. This approach has worked in the past, e.g., in groups of electrical companies coordinated by EPRI.

O. Problems in withholding information from foreign competition and current regulations referring to the handling of proprietary information need revision or the industry participation is academic.

O. Collaboration with foreign firms can be productive, particularly in Dr. Morris' experience with Japanese firms.

O. In the past it has been industry's experience that when working with the Japanese, it was difficult to extract technical information.

O. Certain things need definition like what is an advanced material? It could be an exotic substance, a better steel, or a new coating. The selection of research topics is extremely critical.

O. NCAM needs advice and review from industry to avoid making mistakes in selecting and conducting the program.

O. Industry research of the 50's collapsed because it had little direction. To avoid these mistakes, we need shorter range goals.

O. NCAM must consider not only what programs to start but also criteria to decide when a program should be terminated, both when it is fully successful and when it makes inadequate progress.

Q. Is NCAM's budget the laboratory's total materials research funding?

A. No, LBL's current materials research budget, including funds for chemistry, is approximately $15 million. This is low in comparison with other national laboratories. NCAM's funding will bring LBL to the level of other national laboratories. DOE provides all the funds for materials research at LBL.

O. The present research comprises a large number of separate proposals by individual research investigators, whereas NCAM should include a significantly smaller number of large, interdisciplinary proposals carefully selected for industrial applicability and integrated into a unified program.

Q. What fraction of the operating budget will support education as opposed to product development or patents?

A. It will be split roughly 50-50.

O. The key issue appears to be to identify the two to five problem areas for emphasis in the initial programs.

Mr. Mark Owens, Deputy Division Head of the Administration Division, related LBL's present experience in the patent and data handling area pointed out some of the existing problems regarding patents and data, work for others, collaborative work, protection of proprietary information, indemnity, and pricing policies.

Q. How much work at LBL is currently sponsored by industry?

A. About 15 to 20 contracts.

Q. Have you looked into the possibility of setting up a foundation to own NCAM patents?

A. Not yet.

Mr. Theodore Kirksey, the Laboratory Deputy for Information Services, discussed the current Laboratory Technical Services organization, previous significant technology transfers, and the present procedures for technology transfer.

Q. With joint appointments of personnel between the laboratory and campus, what is the rule when an invention is made?

A. If the invention is made during campus time, patent rights go to the university; if the invention is made on laboratory time, patent rights go to DOE.

Q. How many of LBL's graduate students are foreign?

A. Fewer than 20%.

Q. Is there any research at LBL to which the foreign students do not have access, and is this a problem?

A. This problem has not come up, but it will be an issue with NCAM.

O. The question of foreign nationals will have to be addressed in NCAM, particularly if you get industry involved.

Q. How do other agencies doing work with industry, such as NBS and DOD, handle patents?

A. Each government agency has different patent rules. We are not familiar with NBS but DOD apparently has much looser requirements.

Q. Do you have a policy on technology transfer to foreign agencies?

A. There are no restrictions to distributing information on our current research.

Q. Does DOE have joint patents?

A. Not to our knowledge. In most cases DOE takes title.

Q. Has DOE been approached for delegative authority to release data and patents. Nothing is more discouraging to industry than the present delays.

A. Yes, we have been discussing the subject with DOE for some time. There will be a conference at the DOE Regional Office in June to discuss these issues. Until new policies are set, we must take individual requests and details of proposed cooperative agreements to DOE for approval on a case-by-case basis.

O. The NCAM approach is unique. It is a pioneering effort and the issues are fundamental. There apparently is no model established for this type of relationship, which has industry and a national laboratory working together on research of interest to industry.

O. That is what the workshop is to address. We hope this group produces many suggestions to make the NCAM approach work and points out obstacles and indicates how these obstacles should be negotiated.

In the afternoon, the workshop attendees divided into three groups to develop recommendations.

Group 1	Industry Input on Programs	— Dr.Andrew Kaldor, Leader
Group 2	Proprietary Constraints — Need to Change Existing Regulations	— Dr. Paul Greene, Leader
Group 3	Technology and Personnel Transfer	— Dr. George W. Wiener, Leader

The participants reconvened at 3:30 p.m. to hear the group leaders' reports. Later the leaders submitted written reports, which are attached.

Dr. Kaldor presented the report from Group 1. In the discussion following his report, Dr. Shirley requested advice on the proposed program and the areas NCAM should emphasize, given

that the time-table for the programs to affect industry significantly would be on the order of ten years. Dr. Kaldor indicated the group thought there were currently too many programs proposed. He agreed to poll workshop participants for their specific recommendations on the program, after they have reviewed the NCAM Scientific Program Summary. He suggested that the detailed programs might be defined following workshops addressing key research fields.

Dr. Greene presented the report from Group 2. Discussion following Dr. Greene's presentation focused on the publication delay time required to insure patent registration (domestic and international). Although 6 months to a year might be adequate for this, it may not be enough time for the discoverer to recognize the significance and usefulness of his results. The participants recognized that publication delay is inconvenient to students performing the research as part of their graduate work. However, U.C. already allows a delay of 6 months to allow patents to be filed. In addition mechanisms will need to be devised to prevent overseas transfer of the technology, and to allow proprietary research with reasonable assurance that the work remains secret.

Dr. Weiner presented the findings of Group 3 which were accepted with no discussion.

Dr. Heinemann closed the workshop by thanking the industry participants. He noted that all the working groups seemed to have arrived at the conclusion that selection of the right programs was the major task to be addressed. After some discussion it was decided that a follow-up workshop by this group might be held after the initial programs have been started.

Report from the Working Group on Industry Input on Programs*

U.S. national interests would be well served by new, innovative ways to harness the scientific resources of the National Labs and Universities to develop technologies useful to U.S. industry by making high technology industries more effective and competitive in the international marketplace. The NCAM proposal offers an opportunity to structure and develop fundamentally new institutional arrangements among Industry, Academia, and Government — something substantially different than what is in place now. There is an opportunity, therefore, to utilize NCAM not only as a science laboratory to provide the foundation for the development of new technologies, but that also as a laboratory in which to experiment and develop the sociology and politics of how government and industry may work together toward this end. It is felt that if successful models for such interaction emerge from NCAM, they would benefit, through replication, a much wider sector of the economy than the specific technological achievements alone. There was a general feeling that research programs and organizational arrangements could be developed to insure the success of NCAM, but that much more planning and further discussions are needed to achieve this. The participants felt that this was worth the rather substantial effort required.

The subcommittee began to address the question of how best to organize and formulate industrial input into NCAM's programs. In the process, several important, and unresolved, issues emerged. Some concerned the nature of NCAM: Is it to have primarily technology or science orientation? How much emphasis should be placed on future vs. current technology? Should there be many small programs or few large ones? Other questions also emerged during the initial discussion: What kind of materials are included under NCAM's charter? How broad a sector of U.S. industry does it hope to address at any one time? How does one establish the priority of claims by the industrial sector on NCAM's resources? How does one make NCAM's programs different in character from other LBL programs, and what is the relationship among them? What is the time-scale for NCAM's impact? What is the goal against which NCAM should be judged?

There was agreement among most participants that substantially more discussion is needed to answer these questions and in the process to define NCAM, i.e., what is it about, what is its mission, what are its specific objectives, and how best to attain them. LBL management appears

*Andrew Kaldor, Leader, Praveen Chaudhari, Robert A. Fisher, Michael Korchynsky, Christopher Magee, Alan G. Miller, J. R. Thomas, and J. William Morris, Jr.

very flexible and open in seeking input and advice. But, there is some concern that the sense of urgency and impatience exhibited by NCAM's promoters at LBL is both a compelling indication of commitment to make NCAM work and an indication of a lack of appreciation of the cultural, rather than technical, complexities standing in the way. Just as creative sparks cannot be forced in science, neither can they be forced in the development of new and novel institutions. All one can hope is that the right people are thinking about the problem and are willing to act in concert.

The discussion brought about by the NCAM proposal does provide the climate where creative ideas are likely to emerge. It is worth dwelling on this a bit more. The proposal to develop NCAM originated from LBL with no industrial input to define the need, the approach or the utility. Much of the LBL "industry input" is by faculty or principal investigators who are industrial consultants or had past industrial experience. While these are valuable starting points they do not represent the potential receivers of NCAM's output. Thus the proposal in a general sense is right, but there is little likelihood that it is so in detail and substance.

This workshop served well the purpose of defining the opportunities and issues, and of bringing the industrial participants together to discuss them. But, due to time constraints, it failed to develop the ideas further than to the level of the most obvious conclusions. While much of the discussion so far has focused on changes needed in DOE policy to foster and encourage industrial participation, it has to be recognized that one is dealing only with the symbols of industrial reticence and not its substance. These mechanical and bureaucratic problems will be solved, though with considerable effort. But the sociology of bringing National Laboratories into the picture so that they are a part of the strategic thinking of industrial R&D managers is a much more difficult and diverse problem. At the workshop, none of the industrial participants saw an obvious way that this can be accomplished. It will probably take a prolonged courtship to work the slow process of industrial involvement and commitments. This does not mean that NCAM should wait until all the details are worked out — rather that the number of programs should be reduced and resources focused on a few well defined activities that rapidly validate NCAM's promise. Establishing as soon as possible NCAM's credibility, even in a small way, will have a big impact on assuring the industrial community that this program is substantially different than the standard National Laboratory efforts in this direction. These efforts offer industry the use of special facilities or seek to transfer technology, whether there is a recognized need or not. For example the subcommittee understands that the ALS would and should serve a broader clientele than NCAM; NCAM would be only one of its users, as programmatic needs dictate. Therefore the construction and operation of the ALS should be organized and justified separately from NCAM, otherwise the credibility of the other NCAM promises could be reduced.

The subcommittee discussed how industrial input into NCAM programs and plans may be generated. One important consensus was that advice on program directions by potential users of the science and technology developed by NCAM without some commitment of resources (which may be in terms of time of key scientific personnel rather than direct funding) has to be viewed with a great deal of skepticism. Organizational priorities in industry change, perspectives need to be filtered, etc., and resource commitment guarantees a higher level of review and deeper perspective. Thus, LBL is urged to seek research guidance in such a way that the value of the guidance is scaled by the resource commitment of the organization offering it. Of course, safeguards have to be included to ensure that the advice of small organizations with limited

resources is weighed fairly. One could envision an arrangement that would provide government grants to encourage active participation by small organizations.

Focusing of interdisciplinary science teams in industry usually occurs when a specific problem has to be solved, when a significant science lead has been uncovered and further exploration of that lead is sought, in complex areas where only an interdisciplinary team can make the essential discoveries, or in the early stages of development. One approach for NCAM could be to identify one candidate opportunity in each of these modes and concentrate on them.

LBL should solicit and fund workshops proposed by industrial sources with the avowed purpose of identifying broad areas of scientific interest pertaining to specific areas of technology and with specific R&D potential. The proposals for such workshops should be judged on how broad industrial participation is, how well opportunities for technological transfer are identified, the level of current industrial and academic R&D effort in the area, etc. One outcome of the workshop would be specific NCAM program proposals which have specific industrial resource commitments, input, and review.

LBL should also hold industrial workshops to review basic materials research programs currently at LBL, UC, other National Labs, and other universities. Some of these programs may have the potential to be identified for NCAM focused research activity with industrial participation. The thrust of this effort would be to identify science leads already at hand. This could be an effective way to develop programs with a shorter timescale, especially those formed jointly with industry.

Some areas of potential interest for NCAM programs where workshops should be held were identified by members of the subcommittee. These include ceramics, polymeric composites, alloys, novel metals, polymers, catalytic materials, semiconductors, minerals, coal, and shale, as well as process modeling.

One relationship that was hard for the participants to understand was that between current LBL science programs and NCAM. If NCAM is to be a focused research activity and its science base defined by other LBL activities, then one can see how NCAM can have a shorter range (3–5 years) technology transfer mission. On the other hand, if NCAM is to develop its own long range science programs, then presumably they would be focused and thus different from the other LBL programs already in place.

If NCAM works in the first mode, then it can appeal to and interact with that large section of U.S. industry which, by and large, does little basic science of its own. With these companies, the communication link is in the technology language and the time scale of three to five years for technology transfer matches well. If it is in the second mode, then NCAM will find it easier to interact with organizations that have long-range science programs of their own, mostly larger corporate research labs. Here the time scale of greater than five years is feasible. Industrial input into programs depends strongly on defining this issue.

If a longer range perspective is followed, an important question to address to broad industry groups, such as those in communication and information, energy, chemicals, automotive, steel, etc. would be: what do you see technologically in the 1990's and beyond that threatens your industry? How do advances in materials, or materials processing impact on this threat and how do you plan to deal with it? What kind of organization at LBL would be most useful to you in responding to this threat? One could envision each of these technology areas providing an industrial advisory committee to interact with NCAM on a long term basis.

The subcommittee also considered how NCAM's progress may be measured. One suggestion was to focus on the derivative of industrial participation in a specific program on a five year time scale. If the derivative is positive, it would be viewed as affirmative. Another approach may be to look on the same time scale at industrial involvement in programs in general. Criteria may include whether there are industrial people in residence at NCAM working on the program? Is industry expanding resources to exploit NCAM results? Is industry assessing the opportunities identified by NCAM's program?

We recommend that DOE should only fund NCAM programs after a favorable review of these programs by the affected industrial areas, i.e., the potential customers. We urge that some measures to insure preferential U.S. industrial participation be included in NCAM policies. Finally, to insure small company involvement in the planning and execution of technical programs at NCAM, partial financial support should be available on competitive basis.

Transfer of people from industry to NCAM, on a temporary basis, into technical leadership and even management positions may be another innovative approach to facilitate NCAM's evolution. This is a tricky problem because few organizations can afford to release their best people for extended periods of time, but it is worth pursuing. It may be a career development route.

We think the proposed NCAM program is an exciting, new enterprise well worth considerable effort and support. We would like to make sure that it succeeds and flourishes. The comments above are offered in that spirit.

Report from the Working Group on Proprietary Constraints*

If LBL wants strong industrial participation in NCAM program definition and execution, then modification of DOE policies regarding patent assignments, foreign protection and the protection of technical data is essential.

Certain specific areas were discussed and the following were recommended:

1. *Data* and *technological* disclosure issues for joint ventures of industry and NCAM.
   a. Need *reasonable* time delays for *publication — case* by *case*
   b. Proprietary proposals; How to review without disclosure?
   c. Open laboratory vs. controlled laboratory? Perhaps restrict student access to specific programs.
2. Program policies beneficial to the U.S.
   a. Delay publication for more than 6 months.
   b. Patent as soon as possible — worldwide
   c. Police the patents
   d. DOE policies *require* modification to achieve recommendations 2a, 2b, and 2c.
   e. Require controlled and probably restricted access by *foreign nationals*.
3. *Incentives* for industry monetary participation need to be generated.
   a. Exclusive patent licenses
   b. Royalty differentiation
   c. Other benefits for contributing U. S. companies.
4. Areas requiring legal clarification and perhaps changes.
   a. Antitrust problems — *need legal review.*
   b. Legal roadblocks or concerns regarding the setting up of joint ventures/corporations, re the suggestions in Section 7 of the NCAM Scientific Program Summary.

*Paul E. Greene, Leader, Ralph Dalla Betta, Edward Barlow, Robert E. Hefner, Alexis T. Bell, Stewart Arnold, and Mark Owens, Jr.

Report from the Working Group on Technology and Personnel Transfer*

Each of the industrial members of the group were on the staff of a large central research laboratory. Therefore, the discussion started with the problems of technology transfer within industry. It was generally concluded that technology transfer even within a corporation at times can be very difficult. The problems of technology transfer from NCAM to a heterogeneous industry in which the primary support for the research will come from the government is expected to be a very difficult job. Several factors were identified which are necessary to have successful technology transfer. These factors are:

a. Transfer of people from the operating company to the laboratory and sometimes vice versa.
b. Transfer of part of a project from the laboratory to an operating company R&D group.
c. Have operating groups pay some share of the cost of the R&D program.
d. Ensure a high level of interest between management of the operating company and the R&D projects being undertaken at the laboratory.
e. Ensure continued communication between the laboratory and the operating groups.
f. Oftentimes a champion will emerge and take the risks to see that the technology is transferred.

In considering NCAM, the group concentrated on two items in the above list: item a, people transfer, and item d, to ensure interest by industry in the NCAM program. It was the consensus of the group that it would be necessary for industry to have the option of assigning personnel to projects being carried out at NCAM. Assignments might range from a few months to perhaps as long as a year. It would be expected that industry would maintain the salary and continuity or employment of the assigned personnel, and NCAM would provide all facilities required to do and report on the research project. On general generic research, it would not be expected that industry would pay any money to the NCAM project.

Much discussion centered on how to develop industry interest in NCAM programs. It was agreed that the process of selecting the projects to be undertaken will be a critical factor in determining the extent to which industry will be interested. It was felt by the group that the projects would have to be targeted. The other condition is that the projects before they were established would have to undergo a review process by appropriate industrial representatives before they were established in the NCAM program. The group felt very strongly about this point and agreed that it was a necessary condition if technology transfer were to be successful and meaningful.

*George W. Wiener, Leader, Thomas Clough, C. H. Hamilton, Robert M. White, Heinz Heinemann, and Theodore H. Kirksey, Jr.

NCAM INDUSTRY PARTICIPATION WORKSHOP AGENDA

MAY 23, 1983

(Director's Conference Room - Bldg. 50A, Room 5132)

8:15 am	Bus pickup at the Claremont Hotel	

INTRODUCTORY AND BACKGROUND REMARKS

9:00 am	Welcome and Institutional Overview	D.A. Shirley
9:15 am	NCAM Program Facilities • Present Facilities • Future Facilities	H.A. Grunder
9:30 am	NCAM Science Program Overview	E.E. Haller

INDUSTRY PARTICIPATION

9:45 am	Initial Planning and Procedures for Selecting Research Areas to be Pursued	H. Heinemann
10:00 am	Types of Industry Participation Envisioned • Advisory Groups • Program Collaboration • Scientific Personnel Interchange • Consulting as Required	J.W. Morris
10:15 am	Discussion -- Feasibility, Extent	

JOINT INDUSTRY -- GOVERNMENT PARTICIPATION

11:00 am	Current Experience and Difficulties • Government Goals (Impartiality - Maximum Distribution) • Patent and Copyright Considerations • Reinbursement Requirements	M. Owens
11:15 am	Technology Transfer -- Previous Experience and Present Procedures	T. Kirksey
11:30 am	Discussion re Industry Requirements • Patent, Copyright and Licensing Requirement • Data Publication and Distribution • Handling of Secret and Proprietary Data • Technology Transfer	

	• Personnel Exchange	
12:30 pm	Lunch -- Dr. Shirley's Office	
1:30 pm	Three Working Groups to Define Industry Experience and Recommendations	
	Group 1 -- Industry Input on Programs Group 2 -- Proprietary Constraints, need to change existing regulations Group 3 -- Technology and Personnel Transfer	
3:30 pm	Working Group Leaders' Reports to Assembled Participants	
4:00 pm	Closing Summary and Comments	H. Heinemann
4:30 pm	Bus to Hotel	

PUB-5110

Workshop on the Electronic Materials Program

Lawrence Berkeley Laboratory
October 10–12, 1983

Chairman

Eugene E. Haller

Group Leaders

Robert S. Bauer (Xerox PARC)
Pierre Petroff (Bell Labs., Murray Hill)
August Witt (MIT)
Jerry Woodall (IBM, Yorktown Heights)

February 1984

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

This work was supported by the U.S. Department of Energy
under Contract DE-AC03-76SF00098

Foreword

The Electronic Materials Program Workshop was the first of a series of workshops held at the newly founded Center for Advanced Materials (CAM) at the Lawrence Berkeley Laboratory. Over one hundred attendees from the United States and a few foreign countries came to Berkeley for three days from October 10 to October 12, 1983 to comment on and to provide input to the proposed Electronic Materials Program. Each attendee had ample opportunity to study the proposed program presented in the form of a Discussion Document before coming to Berkeley.

In order to provide appropriate foci for the various aspects of the proposed program, four working groups were formed. The group for GaAs applications was guided by Dr. R. Bauer, Xerox PARC; the group for bulk crystal growth was led by Prof. A. Witt, MIT; the group for thin films and interfaces was headed by Dr. J. Woodall, IBM, Yorktown Heights; and the characterization group was chaired by Dr. P.M. Petroff, Bell Laboratories, Murray Hill. After hearing five plenary talks, which are summarized in this report, the attendees joined the various working groups and listened to special presentations by a number of experts. Ample time for in-depth discussions provided many opportunities to explore the present state of the science and technology of III-V compound semiconductors, primarily GaAs-based compounds. After identifying the near- and long-term problems related to III-V applications, bulk crystal growth, thin films and interfaces, and characterization techniques, the group leaders, supported by local scientific secretaries, summarized their findings and recommendations in their reports. These reports represent the core of the proceedings. The reports were reviewed in draft form by the attendees during the workshop and have been approved in the present form by each group leader. The figures following each group report illustrate some major scientific or technical result, problem, or technique and shall help to illustrate a few aspects of the present state of the art. The workshop has greatly helped the Electronic Materials Program in insuring that the most important problems will be addressed. We are pleased by the broad and strong endorsement reflected in the four group reports of the work which we proposed in our Discussion Document. From the comments of many attendees one can conclude that the workshop will not only have a profound impact on our program but also that it has fostered many useful discussions and contacts between scientists and engineers in this exciting field. We further hope that our colleagues from industry became convinced that we plan to tackle scientific problems of interest to industry and of importance to national needs. We are looking forward to highly productive research in a rapidly advancing field, and we hope that many of the contacts which were made during the workshop will develop into strong fruitful collaborations. Last but not least, we want to thank the management of the Lawrence Berkeley Laboratory and the U.S. Department of Energy for providing the necessary support to start this new exciting program in a truly advanced materials area.

Berkeley, February 1984

Eugene E. Haller
CAM Electronic Materials
Program Leader and
Workshop Chairman

Contents

Foreword v

Summaries of Plenary Talks

- Physics of III-V Compounds 3
- GaAs Technology: A Perspective 7
- GaAs Bulk Crystal Growth 9
- Compound Semiconductor Epitaxy 13
- Deep Defects in GaAs 21

Workshop Reports

- GaAs Applications 25
- Bulk Growth of GaAs 33
- Thin Films and Interfaces 41
- Characterization 47

Workshop Agenda 59

Discussion Document for CAM Program on Electronic Materials 63

List of Attendees 79

SUMMARIES OF PLENARY TALKS

Physics of III-V Compounds*

J.S. Blakemore
Oregon Graduate Center
Beaverton, Oregon

*Work supported by the National Science Foundation, through Grant DMR-8305731.

This talk concentrates on properties of GaAs inherent in its "pure and perfect" zincblende (sphalerite) lattice. Some comments are included on the relation with other III-V semiconductors. As used in technology, GaAs is strongly affected by (intentional *and* inadvertent) native defects and foreign dopants—the concern of several contributions to this workshop program. Knowledge of the "intrinsic" properties, their symmetries and anisotropies, can help assessment of the various extrinsic influences.

The zincblende structure of GaAs occurs also for most other III-V solids (InSb, InP, GaP, etc.), including ternary and quaternary systems such as $Al_xGa_{1-x}As$ and $In_xGa_{1-x}As_yP_{1-y}$. The symmetry limitations of this structure are significant for crystal growth, just as the Brillouin zone geometry delineates possible forms for physical and electronic properties of these cubic (but not perfectly isotropic) solids. Anisotropy of the elastic properties and phonon spectra have possible implications for the stress state of grown crystals. In reviewing "physical" characteristics of GaAs, some lattice thermal properties will also be noted.

The "intrinsic" optical properties of GaAs show two major contrasts with those of a Group IV element. One of these is the steep and strong interband absorption edge, beneficiary of the direct-gap band structure for GaAs (and for several other III-V compounds). The second is the strong coupling of longwave IR (around 37 μm in GaAs) to optical-branch phonons, with attendant strong dispersion, absorption and reflection ("reststrahlen"); all this the consequence of partly polar bonding in any III-V solid. Extrinsic modifications of the optical properties to be noted include: development of a plasma reflection edge when n_o is large, free carrier absorption, photon-induced intraband transitions, and doping effects upon the intrinsic edge.

Comparisons and contrasts of the GaAs band structure with those for Group IV elements will be noted. Thus, the same trio of upper valence maxima are found at the zone center, with effective masses and a spin-orbit splitting all slightly larger than in the isoelectronic analog—germanium. However, the hole mobility in GaAs is considerably smaller than in Ge!

The ordering of the three lowest conduction minima (at Γ, L, and X) for GaAs differs from that in Ge, with consequences much more radical than simply a doubling of ϵ_i. Location of the lowest C.B. minimum at the zone center means, for one thing, that the electron effective mass is small, and almost isotropic (though it *is* energy-dependent, and the "nonparabolicities" of the various zone-center band extrema are interconnected). That small m_e endows a rather high-electron mobility, the principal reason for most current technical interest in GaAs.

There have been many numerical models for the variation of electron ensemble drift velocity versus electric field: steeply rising at first due to the large μ_n, but with a retrograde slope ("Gunn effect") for a field large enough to transfer electrons to lower-mobility upper-C.B. valleys. What happens when an electron mean free path exceeds the gate length in a sub-micron FET? Does ballistic-mode travel then permit velocity overshoot to well above $v_s(max) \sim 2 \times 10^7$ cm/sec of a scattering-stabilized situation? Answers to these questions, when available, will influence the choices of active layer materials and geometries for the highest speed devices.

For the III-V semiconductors with a zone-center lowest C.B. (GaAs, InP, etc.), the resulting *direct* nature of the intrinsic gap means not only a steep and strong intrinsic optical absorption edge, but also full reign for direct interband electron-hole recombination

40-574 O - 85 - 82

mechanisms, both radiative and Auger. Compounded with the proclivity of compound semiconductors to host various kinds of native defects and complexes, large carrier lifetimes and diffusion lengths on the scale customary for silicon can not be expected. That does not preclude bipolar GaAs active devices, but is an extra burden for any developing GaAs bipolar technology (including heterojunction technology) to sustain.

An attractive feature of both GaAs and InP is that ϵ_i is large enough for near-intrinsic material to be semi-insulating at room temperature. How such semi-insulating status can best be provided and maintained in an "inert" substrate form will have much to do with the viability of III-V technology for the larger scales of application.

GaAs Technology: A Perspective

Robert A. Burmeister
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Palo Alto, California

GaAs has electrical, optical, and other physical properties substantially different from those of Si, making it the material of choice for a growing range of semiconductor device applications. It also is of considerable importance as a substrate material for the epitaxial growth of other semiconductor alloys. The overall impact of GaAs technology on the electronics industry has been substantial, and it fulfills a critical role in the development of new fields such as optoelectronics, optical communication, optical memory devices, and ultrahigh-speed integrated circuits. It has clearly become second in importance only to Si as an electronic material.

Important milestones in the evolution of this technology include the development of the halide vapor transport process for epitaxy and the liquid encapsulated Czochralski (LEC) process for substrates, which were developed primarily for light emitting diode fabrication, and secondarily for discrete microwave field effect transistors. Other epitaxial processes including liquid phase epitaxy and molecular beam epitaxy played a key role in subsequent developments.

Within the past few years attention has shifted toward more advanced optoelectronic devices (e.g., semiconductor lasers), advanced high-speed devices (e.g., heterojunction bipolar transistors), and monolithic integrated circuits. In general, these newer devices require GaAs substrates of overall crystal quality at or beyond the present state of the art. This situation has led to increased R&D efforts both in the U.S. and other countries to improve understanding and control of the basic GaAs growth processes.

The current status of bulk GaAs crystal growth technology is characterized by crystal diameters ranging up to 100 mm and boule sizes over 5 kg, but typically having substantial defect concentrations. Dislocation densities in excess of 10^4 cm^{-2} are frequently observed in crystals grown by the LEC process, but somewhat lower values are generally observed for those grown by the horizontal Bridgman process. Several recent studies have attempted to correlate electrical properties and device characteristics with dislocation density and distribution, but the results are not yet definitive. Additional studies have suggested that stoichiometry is a critical parameter which is often not adequately controlled by existing bulk growth processes.

Suggested areas for further research related to GaAs technology include improved crystal growth processes (both bulk and epitaxial), improved materials characterization tools and techniques, studies of the effect of crystal defects on device performance, and improved modeling of material-device interactions.

GaAs Bulk Crystal Growth

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Applications of GaAs for optoelectronics and high-speed microwave devices and circuits place increased requirements on the electrical and structural properties which must be provided, in part, by control over the growth of bulk crystals by solidification from the melt. For minority-carrier devices, such as light-emitting diodes, laser diodes, and photodetectors, a high minority-carrier lifetime and low-defect density is required. For majority-carrier devices, such as MESFETS, a high-resistivity (semi-insulating) substrate is required which is thermally stable. In addition the density of deep energy levels creating generation currents should be minimized. Furthermore for high resistivities to be achieved, the shallow energy levels due to impurities must be compensated by the deep levels which have been reported to be related to non-stoichiometric defects. The integration of discrete devices together on a single chip of GaAs for circuits operating from 3 to 100 GHz and for integrated optoelectronics requires a substantial reduction in defect density from the current value of 10^4 cm^{-2} to levels more typical of silicon technology (1 to 10 cm^{-2}). Furthermore, uniformity of resistivity over both the microscale and chip dimensions is necessary to achieve the desired circuit performance.

Dislocations are undesirable for both classes of devices. In optoelectronics, dislocation arrays can grow into dark-line defects which degrade performance by optical absorption. In microwave devices, dislocations are associated with the defects responsible for the deep energy level, EL2, and which alter the compensation of shallow impurity levels, thus causing large resistivity variations.

Dislocations are generated by thermoelastic stresses, point defect diffusion, and (possibly) self-deformation. The temperature gradients needed in controlling the solidification process are sufficient to cause differential thermal contraction during cooling which gives rise to plastic deformation due to the low value of the critical resolved shear stress (CRSS). At elevated temperatures, dislocation loops may also form by the condensation and collapse of point defect clusters over long periods of time. Lastly, self-deformation may occur because of the low CRSS and high density of GaAs, particularly in the presence of stress enhancement at the outer surface due to notches, B_2O_3 patches, or surface decomposition. The dislocation density can be reduced by lowering thermal gradients in the crystal near the growth interface, reducing the time spent at elevated temperature (increase growth rate), cooling the seed end to raise the CRSS, and by doping the crystal with isovalent Group III elements (with distribution coefficients less than one) to raise CRSS. However, for doping, compositional uniformity cannot be achieved because of segregation effects. The current dislocation density is typically 10^3 cm^{-2} in crystals grown by the horizontal Bridgman (HB) method and over 10^4 cm^{-2} for the liquid encapsulated Czochralski (LEC) method. Lower values have been reported, especially for smaller crystal sizes (2 inches or less). However, scaling up from 2- to 4-in. LEC crystals does not appear to increase dislocation density or distribution very much.

Stoichiometry effects in GaAs bulk crystal growth have only been uncovered recently. It has been shown that melt stoichiometry controls the electrical compensation of shallow impurity levels through the EL2 deep energy level, with higher As melt concentrations resulting in higher EL2 levels and consequently higher "undoped" resistivities. However, models explaining EL2 by invoking various non-stoichiometric antisite defects have been confounded by important experimental differences in contamination between HB and LEC crystals. Furthermore, the degree of As_4 vapor pressure control may not be adequate to provide reproducible crystal stoichiometry control, although this clearly needs to be

resolved by more careful experimentation. It has been observed that infrared absorption ($0.8\ eV < h\nu < 1.3\ eV$) occurs because of the EL2 level. As a result,a correlation of high EL2 concentrations with the presence of dislocations has been possible. It has recently been observed also that the EL2 concentration decreased from $1.2 \times 10^{16}\ cm^{-3}$ to $1.3 \times 10^{15}\ cm^{-3}$ by magnetic field damping of melt convection in LEC. It has also been reported that increases in the pull speed of the crystal tend to increase EL2. However, there is no explanation for such effects.

Impurity contamination effects are very significant in the melt growth of GaAs. When quartz boats or crucibles are used, both Si and O dissolve in the melt and are incorporated into the crystal at levels of $\simeq 10^{16}\ cm^{-3}$. Electrical compensation is achieved by adding Cr to the melts so as to grow semi-insulating crystals for FET applications. In LEC growth, the use of pyrolitic boron nitride crucibles reduces [Si] to $5 \times 10^{14}\ cm^{-3}$. It has also been observed that a further reduction in Si concentrations can be achieved by bubbling of the B_2O_3 encapsulant by means of an abrupt argon pressure reduction. An additional factor affecting the dissolution of quartz crucibles is the water content of the B_2O_3; concentrations below 250 ppm apparently enhance the dissolution rate. (However, higher water concentrations cause twinning of the crystal due to oxide formation.) Additional contaminants include C at concentrations of 10^{15} to $10^{16}\ cm^{-3}$ (an important shallow acceptor) and B (10^{16} to $10^{17}\ cm^{-3}$) for which electrical or structural behavior has not been determined. The role of O (added as Ga_2O) has similarly not been uniquely determined. Analytical methods such as SIMS will require enhancement through the use of the O^{18} isotope to resolve this situation. It is desired to keep all impurities below $10^{14}\ cm^{-3}$ to grow semi-insulating crystals of appropriate resistivity and uniformity.

Compositional segregation effects are very important because the spatial distributions of stoichiometric ratio, impurities, dopants, and isovalent Group III additions are uniquely determined by such effects. For example, where compensation is required to produce high resistivity, the concentrations of both EL2 and shallow impurity acceptors must be separately controlled to produce uniform compensation, perhaps a physico-chemical impossibility. Segregation effects include macrosegregation (due to axial normal freezing distribution and lateral variations due to nonuniform melt convective flows) and microsegregation (due to growth rate fluctuations and constitutional supercooling at higher concentration levels). These phenomena can be controlled to some extent by using forced convection on the one hand and magnetic field damping of thermal convection on the other.

Control methodologies for the melt growth of GaAs are becoming a critical factor because of the increasingly lower temperature gradients required for low dislocation growth. In the LEC method, diameter control has been achieved by meniscus sensing with X-radiography and video-beam blanking methods, by crystal or melt weighing with tared electrobalances or transducers, and by the use of coracles on the upper melt surface to constrain the meniscus position. Of these methods, weighing is the most advanced, and current efforts are being devoted to converting it from analog to digital control methods. If fully implemented as a nonlinear digital control method, it should be possible to achieve full growth control from seed to tail.

Further control over stoichiometry during growth by direct communication of a well-controlled arsenic vapor pressure source with the melt itself is also seen as an increasingly important capability. Such effects have been demonstrated in HB growth but the interpretation has been made difficult by uncontrolled impurity effects.

Future trends and needs in GaAs bulk crystal growth will focus on both HB and LEC methods through scale-up and control of growth to achieve desired crystal properties (orientation, size, electrical resistivity, dislocation density, contamination levels, stoichiometry control, dopant uniformity). Studies of crystal growth conditions will be undertaken using numerical simulation and experimental modeling. Fully instrumented growth will include temperature profiling, convection monitoring, vapor pressure control, magnetic damping, forced convection control of thermal convection effects, and heat pipe or segmented heater control of the melt and solid temperature distribution. The thermophysical properties of B_2O_3 and molten GaAs must be determined (viscosity, surface tension, thermal conductivity, both radiative and normal).

Crystal properties will receive increasing attention. The structural and chemical nature of deep level defects will be explored using more careful thermochemical methods and more advanced characterization techniques. The relevance of dislocations and crystal growth conditions to deep energy level formation will be explored. The nature of the electrical compensation between shallow and deep energy levels, which give the high resistivity so essential to MESFET operation, will be pursued. Dislocation generation mechanisms will be studied and the CRSS measured as a function of temperature and solute additions. The roles of stoichiometry, solute hardening, and strain-rate effects will be studied in detail.

Lastly new growth methods must be evaluated. For example, zone methods such as horizontal levitation and vertical floating zone techniques offer advantages in control of properties that will be useful for research purposes. Also, nearly isothermal bulk growth methods such as Kyropoulos and electroepitaxy may provide baseline data on the role of temperature gradients and thermoelastic stresses in dislocation and defect formation.

Compound Semiconductor Epitaxy

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Interest in III-V compounds stemmed originally from the availability of direct bandgaps, a variety of bandgap energies, high mobilities, and ease of p-n junction formation. By the late 60's it was also evident that the use of crystalline solid solutions to achieve lattice matched heterojunction would permit single crystal structures with large changes in composition, and thus properties, without defects due to excessive strain. The earliest embodiments of such structures were single and double heterostructure lasers, made by liquid phase epitaxy (LPE). Successful demonstration of such devices and subsequent development of epitaxial methods that permit the fabrication of extremely thin layers have caused a rapid increase in interest in III-V compounds and their epitaxy in the last five years. A review of the currently most important epitaxy systems is given.

Liquid phase epitaxy is based on the idea that in systems in which the compound (AB) can be grown from solution rich in one component, precipitation can be made to occur on a substrate seed. Binary compounds are the simplest cases, but the same principle holds for more complex systems such as $Al_xGa_{1-x}As$ on GaAs, and even $InP/Ga_xIn_{1-x}As_yP_{1-y}$.

In spite of the large degree of success with LPE for producing laser structures in particular, LPE has serious limitations. These are: nonuniformity and non-reproducibility, layer thinness limitations, interface grading, and miscibility gaps. Interface grading is thermodynamically driven by the nonequilibrium of a binary substrate seed (for instance) being brought into contact with a ternary liquid phase. Miscibility gaps are expected to be more limiting on a near-equilibrium technique like LPE than other techniques.

Chemical vapor deposition (CVD) (halide transport) utilizes the basic reaction shown in the following equation:

$$As_4(g) + 4GaCl(g) + 2H_2(g) \rightleftharpoons 4GaAs(g) + 4HCl.$$

Arsenic (As_4) can be introduced either as halide ($AsCl_3$) or as hydride (AsH_3). This epitaxial method is useful for single binary layers and for $GaAs_xP_{1-x}$ LED's, but probably not for $InP/Ga_xIn_{1-x}P_yAs_{1-y}$ because of complex boundary layer problems. It will not work for Al-containing compounds due to distribution coefficient and reactivity problems.

Molecular beam epitaxy (MBE) and organometallic chemical vapor disposition (OMCVD) are capable of very abrupt, ultrathin, very reproducible layer structures in $GaAs\text{-}Al_xGa_{1-x}As$. MBE is a UHV technique in which beams of atoms and molecules impinge on a heated substrate. A typical MBE growth chamber is schematically shown in Fig. 1. Epitaxy occurs because one group V atom sticks for each excess group III atom on the surface and because at the growth temperature there is sufficient surface mobility for the atoms to find their lowest energy lattice sites. OMCVD utilizes the reaction:

$$M_{III}R_3 + M_VR_3' \rightarrow M_{III}M_V + R + R'.$$

Results achieved with $GaAs\text{-}Al_xGa_{1-x}As$ are similar to those with MBE. Presumably, in both methods, smoothing to virtually an atomically smooth surface occurs upon growth of an initial buffer layer. The illustrations in Fig. 2 are for MBE samples showing: (a) electron diffraction and SEM pictures of a polished surface, (b) one with several hundred angstroms of GaAs growth, and (c) one with several thousand angstroms of GaAs growth.

Several devices are used as examples to show the superiority of the device performance grown by MBE and OMCVD and the unique capability of MBE and OMCVD to grow novel device structures. For example, injection lasers utilizing multiple quantum wells show very low-threshold current densities (J_{th}), and graded-index quantum-well lasers which are made possible by MBE have similarly low J_{th}. Improved J_{th} occurs in the MQW laser in spite of a multiplicity of interfaces.

Two examples of novel barrier structures fabricated by MBE are the saw-tooth (graded-gap) barrier and the heavily doped thin region (~50 Å). The latter structure, illustrated in Fig. 3, is used in a novel detector in which trapped holes at the gate modulate the barrier height and thus the diffusion of carriers over the barrier. Such a barrier detector is capable of very high-speed operations.

Single interface quantum wells with modulation doping represent a novel structure capable of yielding extraordinarily high mobility as the result of separation of the impurity donor atoms (put into the $Al_xGa_{1-x}As$) from the electrons. Measured mobilities in such structures have improved dramatically as shown in Fig. 4. For comparison, the mobility in an undoped VPE-grown film is also shown.

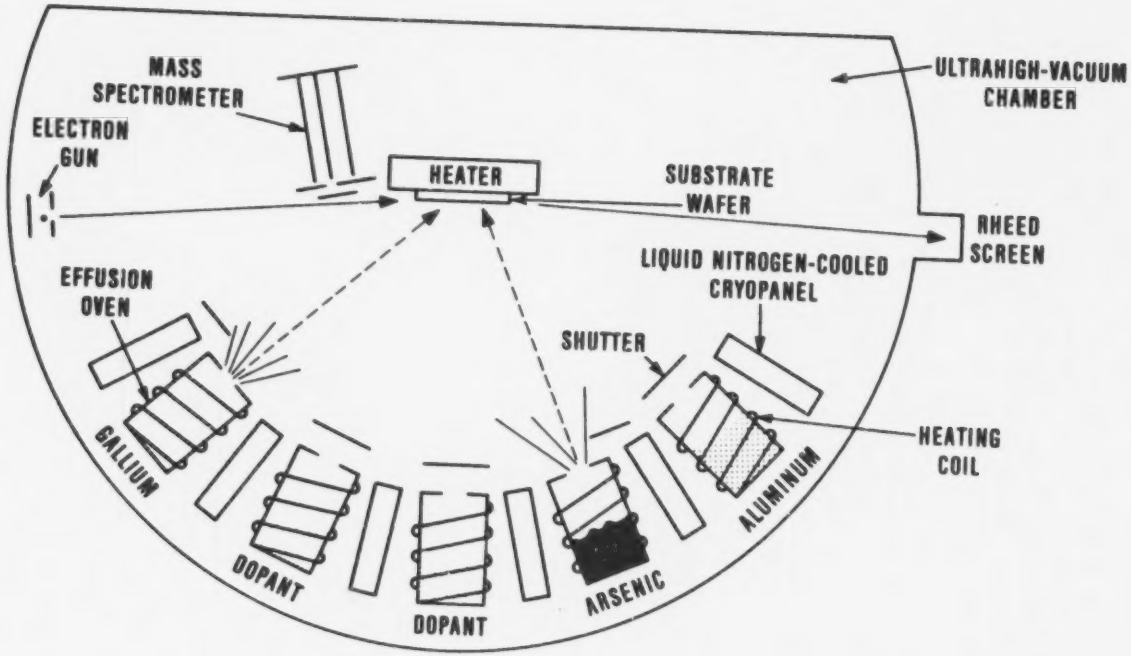

Figure 1. Schematic diagram showing the layout in a typical MBE growth chamber.

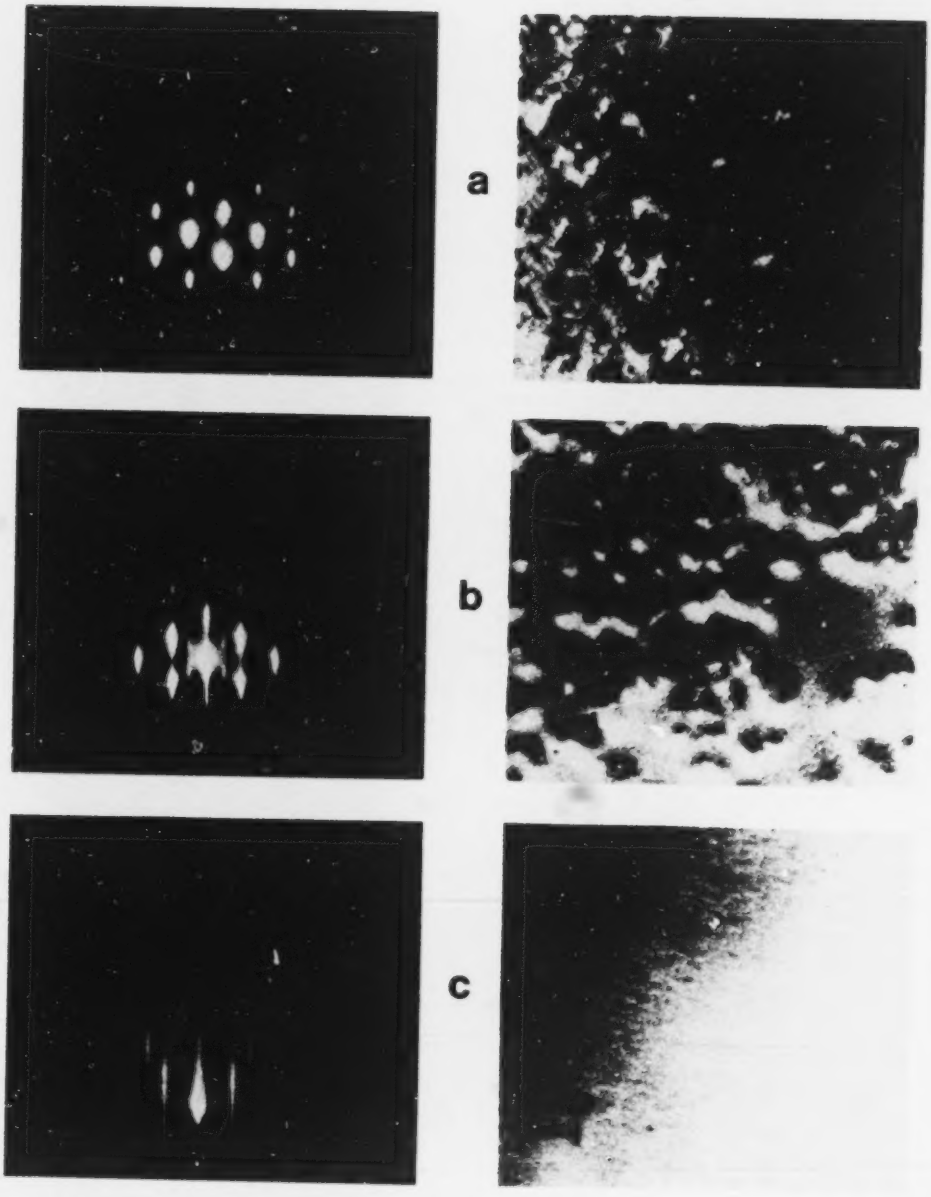

Figure 2. (a) Electron diffraction (left) and SEM photographs (right) of a polished GaAs substrate surface. (b) One with several hundred angstroms of GaAs-MBE growth. (c) One with several thousands angstroms of GaAs-MBE growth.

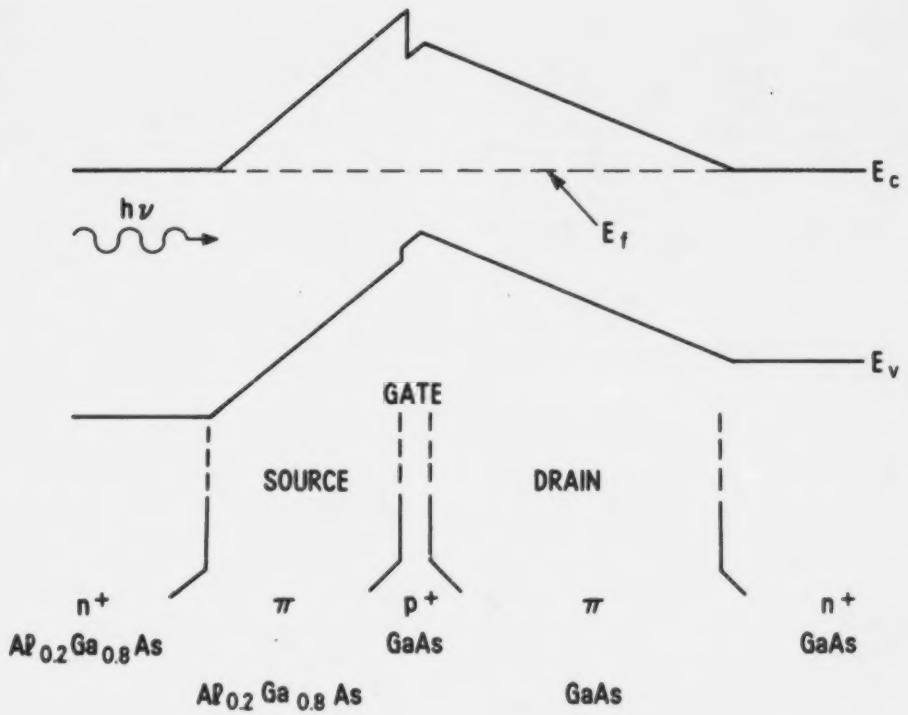

Figure 3. Band structure of a novel photon detector FET.

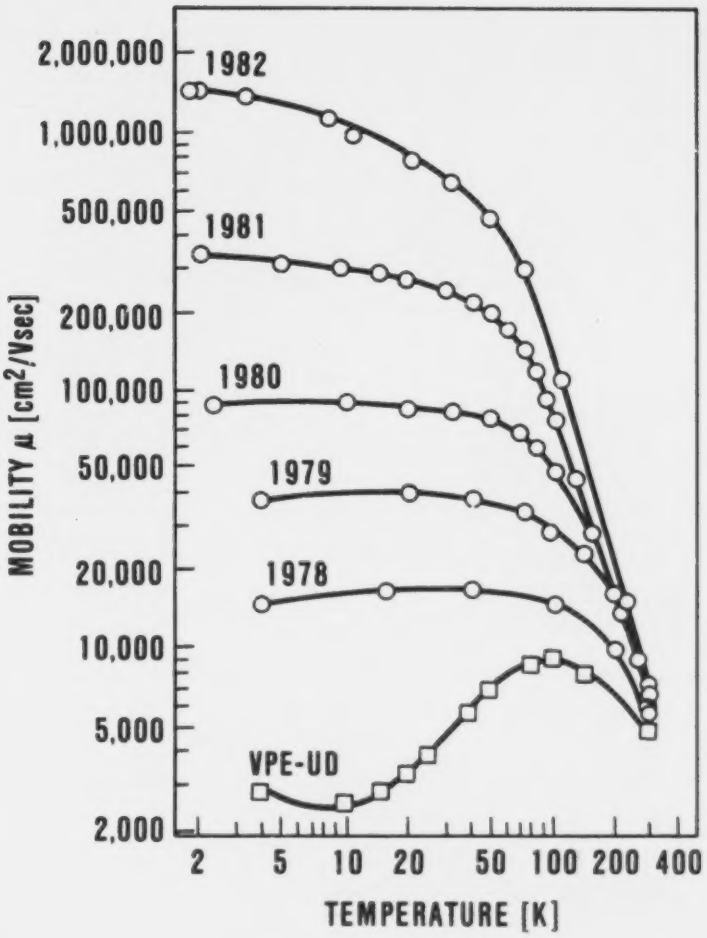

Figure 4. Improvement of carrier mobility in quantum-well structures over the past six years. A high-quality vapor phase epitaxy (VPE) layer shows a substantially lower mobility.

Deep Defects in GaAs

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Freiburg, W. Germany

A survey is given on the electronic structure of "deep" defects in GaAs. Such defects play a vital role in the compensation processes occurring in semi-insulating (s.i.) GaAs. Defect structures to be discussed are 3d-transition metals and stoichiometric defects, in particular, As_{Ga} antisite defects.

3d-transition metals in GaAs have been extensively studied by electrical methods as well as by optical and ESR spectroscopy. From this it became apparent that they form deep acceptor states in GaAs, as well as in GaP and InP, when occupying isolated substitutional cation sites. For nickel in GaAs, double acceptor behavior was also detected, as well as a strong tendency for association with shallow group-IV and group-VI donors.

The case of chromium deserves special attention, since the Cr-acceptor level happens to lie near mid-gap. This enables the growth of s.i. GaAs from SiO_2 crucibles, since the deep Cr-acceptor compensates shallow impurity donors such as silicon. On the other hand, substitutional chromium in GaAs has been found from ESR experiments to be an ambivalent dopant, since it also introduces a deep donor level. Such behavior could not be observed for other 3d-ions.

More recently, LEC-growth of GaAs from pyrolytic boron nitride (pBN) crucibles is of increasing importance. In contrast to SiO_2 crucible crystal growth, no shallow donor contaminations from the pBN crucible walls are expected to occur. However, such material is found to be contaminated with carbon impurities, which act as shallow acceptors when occupying As-sites. Consequently, controlled introduction of a deep mid-gap donor level is necessary, in order to render the material semi-insulating. The mid-gap donor level labeled EL2, dominant in such material, has been extensively studied by DLTS and related techniques. Since its creation does not require foreign atom doping, it was assigned as a stoichiometric defect. Furthermore, since formation of EL2 is favored under As-rich conditions of crystal growth, this level is now widely believed to be related to an As_{Ga} antisite type defect.

Antisite defects represent a very characteristic type of lattice disorder in III-V semiconductors. The anion-on-cation site antisite defect, P_{Ga} and As_{Ga}, has been detected by ESR in GaP and GaAs, respectively. In as-grown LEC-GaAs its concentration ranges up to $5 \times 10^{16} cm^{-3}$. Fast electron and in particular fast neutron irradiation, as well as plastic deformation, can increase the concentration of the As_{Ga} defects in GaAs considerably.

From photo-ESR experiments, the energy levels of the As_{Ga} double donor were determined as $E_c - 0.77$ eV and $E_v + 0.52$ eV. Thus, the first level, (D^0/D^+), is very close to that of the EL2 defect. Furthermore, it is noted that the above energies coincide with the Fermi level pinning energies at GaAs surfaces.

So far, no ESR evidence for the complementary antisite defect Ga_{As} could be obtained, although this acceptor-type defect is likely to exist in material grown under Ga-rich conditions. Equally unsuccessful were attempts to identify simple vacancy-related defects, as V_{As} or V_{Ga}, by ESR, although DLTS detection of such centers was reported already a decade ago in fast electron irradiated GaAs.

40-574 O - 85 - 83

WORKSHOP REPORTS

GaAs Applications

Robert Bauer (Xerox PARC) and John Freeouf (IBM Yorktown), Group Leaders
Nabil Amer (LBL), Scientific Secretary

Invited Speakers

- R. Burnham (Xerox PARC): "Multiquantum Well Lasers by MOCVD"
- R. Eden (GigaBit Logic, Inc.): "Applications and Materials Implications for Commercial GaAs ICs"
- L. Eastman (Cornell): "Compound Semiconductor Materials for High-Speed Applications"

Overview

Close cooperation between LBL and industrial research institutions must be a prime management goal of a program in electronic materials if national needs are to be met. Such cooperation will enable the proper research topics to be chosen, based on the experience of industrial experts who understand the problems of an applications-driven environment.

Thus, for example, the identified need for extreme materials uniformity focuses attention on particular types of research, namely, on the bulk GaAs itself, on epilayer growth, and on processing techniques. Such applications require an understanding of the fundamentals of defects and their variation with materials environment (e.g., the anneal temperature), as well as of the scientific basis for epitaxial growth of III-V semiconductors by such methods as molecular beam epitaxy (MBE) and organometallic vapor-phase epitaxy (OMVPE).

The workshop heard from leading experts in the fields of optoelectronics, integrated circuits, and high-speed microwave devices. These three applications areas represent important research challenges that are summarized below. Although progress has been slow, we are now at the juncture where dramatic growth in GaAs devices is expected. This suggests that there will soon be a critical shortage of students trained in the materials science needed for emerging technologies. We are faced with abrogating the opportunity for the United States to achieve a foothold in the rich GaAs field if we do not adequately fund research and training in areas of fundamental importance to such technologies.

Advances in GaAs applications are clearly limited by our lack of understanding and control of materials technologies. We find, for example, that GaAs produced by the liquid-encapsulation Czochralski (LEC) method is so poorly controlled that neighboring wafers from the same boule must be individually characterized and tailored by the ion implantation in order to obtain satisfactory IC performance. The MBE and OMVPE methods are producing impressive results but are limited by defects, thickness nonuniformity, and non-reproducibility of dopant concentrations. Such observations by experts in the field underscore the need for vigorous advanced materials research that is coupled to the experiences of American industry.

Applications-Driven Basic Materials Research Opportunities

Bulk GaAs

In realizing integrated circuits, the properties of bulk GaAs are much more important than in the analogous case of the properties of bulk Si. The reason is related to the use of devices produced by direct ion implantation into the GaAs substrate. Commercial plans for depletion-mode devices are faced with serious problems of threshold nonuniformity. This and similar issues preclude consideration of the more useful enhancement/depletion circuitry, which is now the heart of the production needs for commercial and military high-speed, radiation-hardened, low-power circuitry. Yet in the United States there are no programs aimed at understanding the fundamentals of the materials growth and properties.

We need to study the defects that cause the semi-insulating behavior of the substrates (e.g., the origin of EL2) and to understand the materials-processing effects that allow gettering procedures to be developed. Such research should include a carefully controlled, in-house, single-crystal growth program. There must be strong interaction between the crystal-growth and characterization efforts of CAM. Also, effort should be directed toward developing an *in situ* monitoring technology. A statistical basis for choosing "good" vs. "bad" material could be achieved by in-house characterization of wafers from batches that were then processed and evaluated by industry.

Epitaxial Growth

A fundamental understanding of epitaxial growth is essential for pursuing advanced GaAs applications. Successful commercialization of laboratory devices such as modulation-doped field-effect transistors (MODFETs) and heterojunction bipolars depends on the growth of epitaxial layers of sufficient quality, uniformity, and dopant reproducibility. Furthermore, the effects of substrate quality on epilayer quality require a better understanding.

A research program focused on the fundamentals of epitaxial growth processes should have a high priority. In the MBE technique, the ultrahigh-vacuum environment used for the growth would provide a simple case for scientific inquiry into the basis of epitaxy. In fact, molecular species interacting on surfaces under conditions far from equilibrium provide a unique scientific opportunity for experimentalist and theorist alike. The OMVPE reactor is one of those "black boxes" that have been employed with great success, yet the basic chemistry and fluid dynamics are mysteries that have not yet been explored. Such research would lead to valuable information and would provide a training ground for young scientists and engineers who are vital to American industry.

Compound Semiconductor Processing

The interactions of compound semiconductors with other substances and with perturbing environments (e.g., particle beams or temperature variations) provide a fruitful area for research. By far the greatest failures presently experienced in device production are process-related rather than attributable to the starting material itself. Processes such as ion implantation and activation by annealing are little studied and less understood.

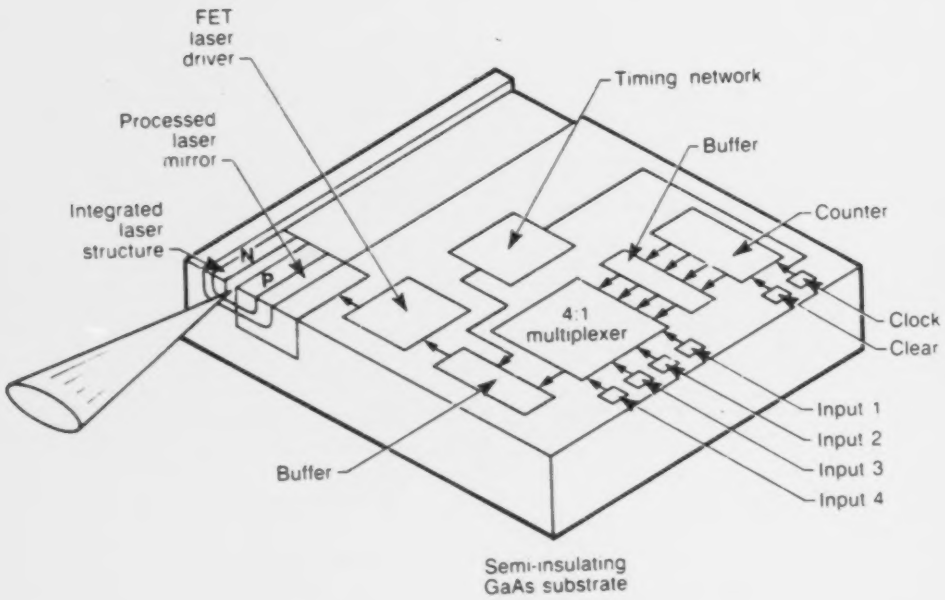
Investigating the reason for the advantage of using an As overpressure during the anneal of implantation damage is an example of a basic research problem that would significantly affect the application of GaAs as an electronic material. We must control the presence and migration of impurities such as transition metals if we are to realize the potential of III-V materials. Accomplishing the latter necessitates small dimensions so that the transit times of carriers are minimized.

CAM's access to synchrotron radiation facilities at Stanford and possibly at LBL could be most valuable for studying the interactions of radiation with organic materials used for photoresists, as well as for studying the x-ray optics necessary to achieve 0.5-μm and smaller features in GaAs. While this may seem tangential to "advanced materials" research, it is closely tied to our ability to exploit the high-speed microwave and IC potentials of III-V materials. Furthermore, such research could foster strong ties between LBL and the semiconductor industry.

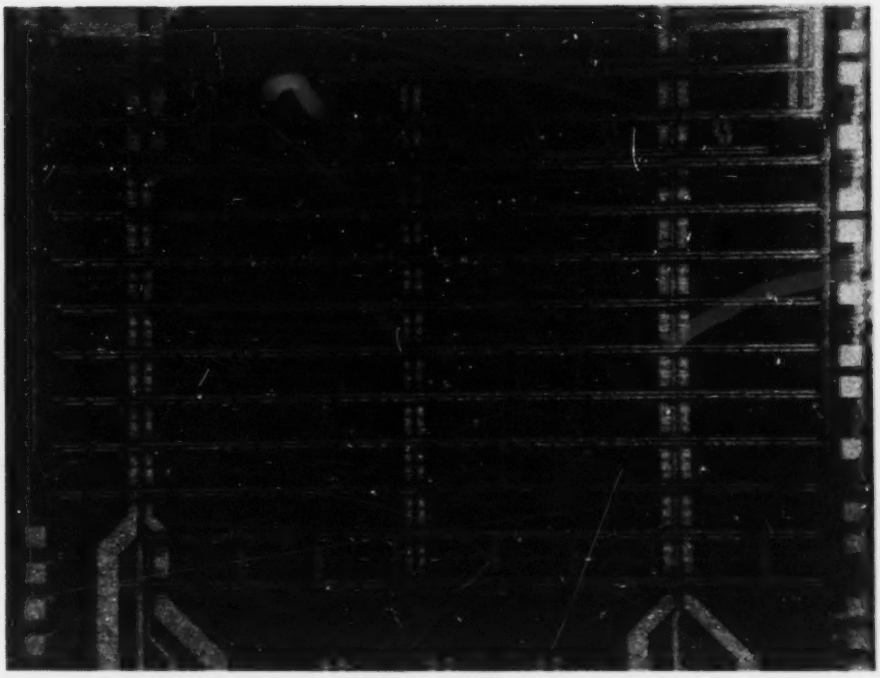
Summary

The national technological base requires that a vigorous, long-term research program be conducted in collaboration with American industry. The Lawrence Berkeley Laboratory could play a pivotal role in this process by creating a partnership with high-technology companies and a leading university. The benefits of conducting basic research on III-V materials will accrue both from the knowledge learned and the personnel trained. Although our graduate programs in advanced materials characterization techniques are adequate, we currently lack adequate programs in materials growth and processing.

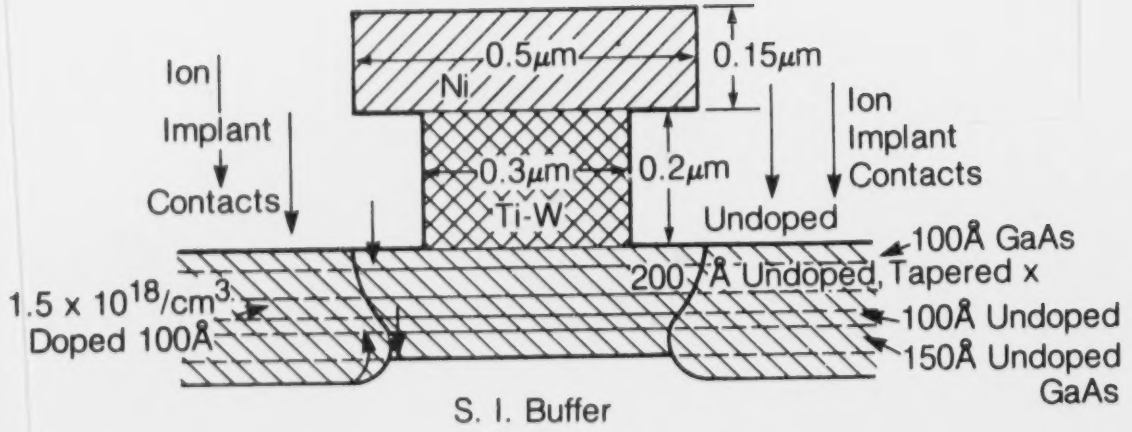
Contributions to our understanding of bulk materials, epitaxial growth processes, and the effects of environmental changes on the materials are vital if we are to have a role in the emerging applications of GaAs. Novel capabilities such as ultrasmall-scale lithography using synchrotron radiation may provide the unique advantage that is needed for the United States to take the lead in this electronics and optoelectronics arena.



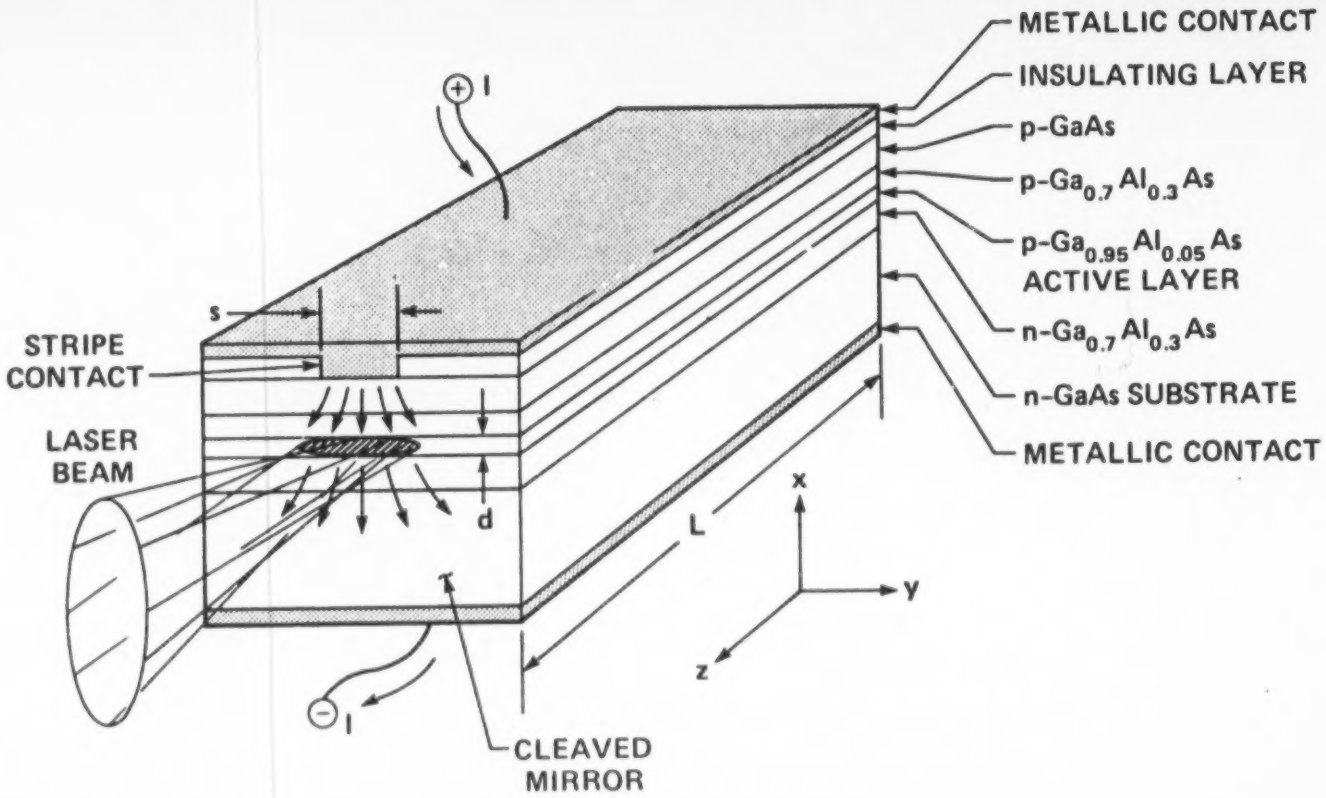
Proposed optoelectronic device reflecting future directions in III-V technology. (After Carney *et al.*, GaAs IC Symposium, 1982)



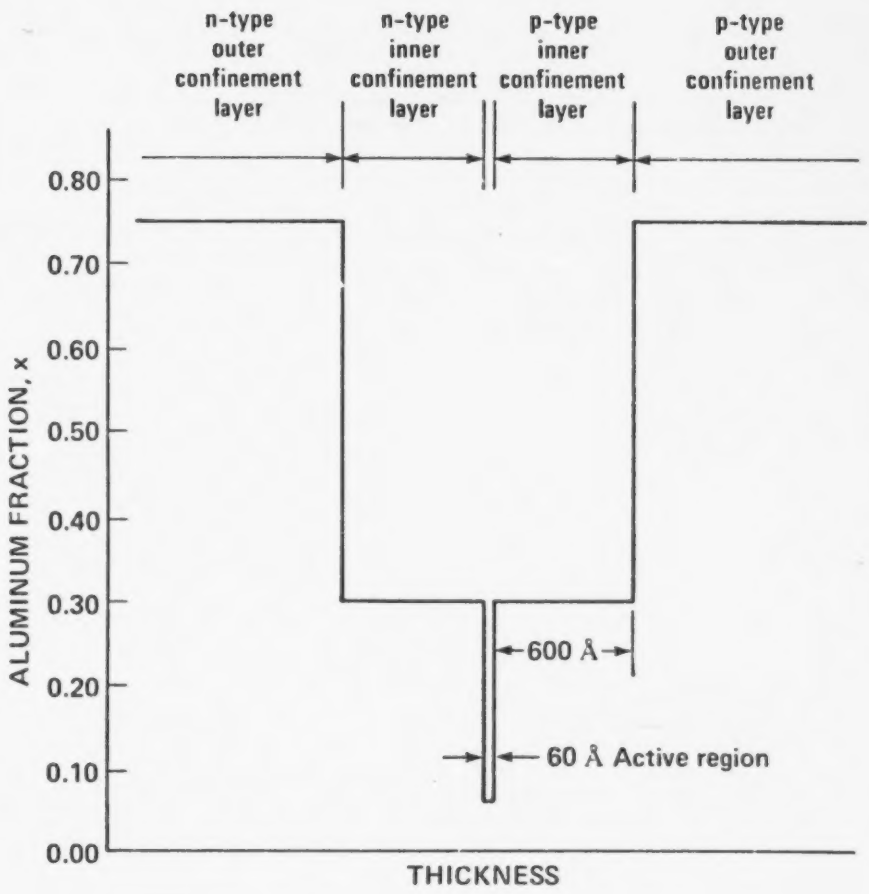
An 8 × 8 bit parallel multiplier with input and output latches, simple ripple-multiplication architecture. The 1008 logic gates of the Schottky diode FET logic (SDFL) type employing one transistor, 2 active loads, and 2–4 diodes per gate. The transistors are normally "On" MESFETS with 1 μm gates fabricated by ion implantation into a semi-insulating GaAs substrate. (Courtesy of R. Zucca, Rockwell International)



Short quantum well MODFET. (Courtesy of L. Eastman, Cornell U.)



Double heterostructure quantum well laser. (Courtesy of R. Burnham, Xerox PARC)



Separate confinement quantum well laser structure. (Courtesy of R. Burnham, Xerox PARC)

Bulk Growth of GaAs

August Witt (MIT), Group Leader
Boris Rubinsky (LBL and UC Berkeley), Scientific Secretary

Invited Speakers

- D.L. Barrett (Westinghouse): "High-Pressure LEC Growth of GaAs"
- A. Jordan (BTL): "Defect Formation due to Thermal Stresses in LEC Growth of GaAs"
- W. Langlois (IBM): "Fluid Dynamics in LEC Growth"
- D. Miller (Airtron): "Low-Pressure LEC Growth of GaAs"
- J. Vaughan (M/A-Com): "Horizontal Bridgman Growth of GaAs"

The contents of this section have come from presentations and extensive discussions at the working group session, in which about 35 scientists and engineers from industry, the government, and academia took part. Further input came from various other sessions.

Current Status of the Field

It is generally acknowledged that the basic property requirements of GaAs for emerging device technologies are met only marginally in material produced with established crystal-growth techniques and that the projected property requirements will probably not be met without significant advances in growth technology. The primary industrial methods for growing bulk GaAs—liquid-encapsulated Czochralski (LEC) growth and horizontal Bridgman growth—are still empirical, without a firm scientific foundation.

Material produced by Bridgman growth is of adequate crystalline and chemical quality for discrete optoelectronic and microwave devices, but many consider it inadequate for the emerging monolithic GaAs IC technology. The basic materials requirement for this technology—undoped semi-insulating GaAs crystals of 3-in. diameter—is met in principle with liquid-encapsulated Czochralski growth. At present, however, diameter control is deficient; purity control, compositional uniformity in the axial and radial directions, and reproducibility are limited; and line-defect densities are excessive.

Recent research has established that, in principle, the two major techniques for growing GaAs permit the control or elimination of present materials deficiencies. Neither of these techniques in its present form is even remotely optimized, however. For example, both of them lack heat-transfer control (thermal gradient control), which is now recognized as strongly affecting the crystalline and chemical quality of GaAs.

Crystal-growth technology, the basis for solid-state device fabrication, must be placed on a firm scientific foundation if it is to meet the demands of projected devices. Achieving this goal will require a coordinated interdisciplinary program of both science and engineering. The Center for Advanced Materials appears to be in a unique position to meet this requirement. A comprehensive effort aimed at optimizing the techniques for growing single crystals of compound semiconductors (specifically, GaAs) can solve important problems in device technology. It will also provide advanced training to graduate students and facilitate their rapid entry into industrial research and development.

Recommended R & D for Bulk Growth of GaAs

It is recommended that the existing growth techniques be comprehensively analyzed for their potential to produce GaAs with a degree of crystalline and chemical quality that is suitable for use in *projected* device technology. This analysis should include but not be restricted to LEC and horizontal Bridgman growth. It should include considerations of the control of thermal gradients in the liquid and crystalline phases, the control of growth-interface morphology, the control of convective flows, the maximum achievable crystal diameter, and the possibility of *in situ* analysis of growth behavior. In addition, the possibility (and merits) of *in situ* synthesis and the related analysis and control of stoichiometry should be investigated.

This study should lead to the identification of one or two growth techniques that have the potential of meeting all projected processing requirements, including wafer diameter. It is expected that substantive elements of the identified system will be commercially unavailable and will have to be developed in-house or on custom order.

The following sections describe the specific theoretical and experimental studies that are recommended.

Theoretical Studies

(a) *Formation of dislocations due to thermal stresses.* (This study should be conducted if LEC is one of the growth techniques selected or if the technique selected is susceptible to stress-induced defect formation.) Emphasis in this study should be placed on the use of realistic boundary conditions approaching those encountered during growth. If possible, the approach should be iterative, making use of such factors as measured temperature profiles, measured dislocation densities, and external crystal morphologies. The study should also consider the dislocation dynamics during growth and post-growth cooling, as well as the interaction of stress-induced dislocations with native growth dislocations. The analysis should lead to the identification of thermal gradient configurations under which slip phenomena are minimized. This study should be conducted for the various growth directions generally employed.

(b) *Formation of dislocations due to other effects.* Limited studies suggest that the conventional Dash approach to the elimination of growth-induced dislocations is ineffective in LEC growth. Since control over the generation of dislocations is a desirable (if not necessary) feature, their origin and characteristics in GaAs should be explored.

(c) *Buoyancy-driven flows and forced convection in the melt.* To a significant extent, convective melt flows and the related heat and mass transfer control the crystalline and chemical quality of the grown crystal. It is therefore essential that a comprehensive flow analysis be conducted and that the results function as a basis for efforts aimed at optimizing the growth conditions. The analysis should be based on realistic boundary conditions, including the existence of encapsulating fluids and the ambient gas phase, and it should account for the effects of applied transverse and/or vertical magnetic fields. The studies of convective flow behavior should enable the identification of rotational parameters leading to minimized radial segregation and to the elimination of both rotational and nonrotational segregation effects. It should also clarify the effects of high-viscosity fluid encapsulants on the boundary layer configuration at the crystal-melt interface.

Experimental Studies

A multitude of essential experimental studies depend on the particular growth method in question and do not need amplification here. In addition, the effects of bulk defects on device properties are presently the subject of extensive studies, so that related experimental investigations cannot be specified at this time. Key experiments aimed at clarifying the formation of the EL2 defect should be postponed. The following is a selection of studies considered important in the present context.

(a) *Solid solution hardening in GaAs.* Recently, substitutional incorporation of isovalent elements has been found to be an effective means for reducing the density of both growth- and stress-induced dislocations. A systematic study involving elements of the

III, IV, and V groups and double doping should be considered. In particular, the yield stress at elevated temperature should be investigated for different dopants as a function of concentration. As part of this study, the effects of solid solution hardening on the electrical properties and on implant properties should be investigated.

(b) *Chemical effects related to liquid encapsulation.* Liquid encapsulation with B_2O_3, although extensively practiced and found to be deficient in various ways, has not yet been systematically investigated. Neither the physical properties (e.g., the optical and thermophysical properties and their changes with continuing growth) nor the chemical properties (interaction with the melt, interaction with the crucible, effect of traces of H_2O on both interactions) are adequately known. A comprehensive study of B_2O_3 and suitable alternates as liquid encapsulants is strongly suggested.

(c) *Crucible materials for GaAs growth.* Both of the conventional crucible materials, pBN and SiO_2, are known to interact, to varying degrees, with GaAs melts and with B_2O_3. As yet the chemistry of interaction is unknown in detail, and only limited research on controlling the rate of interaction has been conducted. It appears essential that the nature of these interactions be quantitatively investigated and that alternative crucible materials be considered.

(d) *Heat transfer control in the liquid phase and the growing crystal.* Major efforts should be made to bring about control of heat flow in the growth system. The focus should be on establishing the axial thermal field distribution and controlling the radial and axial thermal gradients in the vicinity of the growth interface. In pursuing this goal, attention should be paid to high-temperature heat-pipe technology. Considering the importance of heat-flow control during growth and even after growth (along the crystal), efforts should be made to explore available approaches for this purpose, as well as to develop new ones.

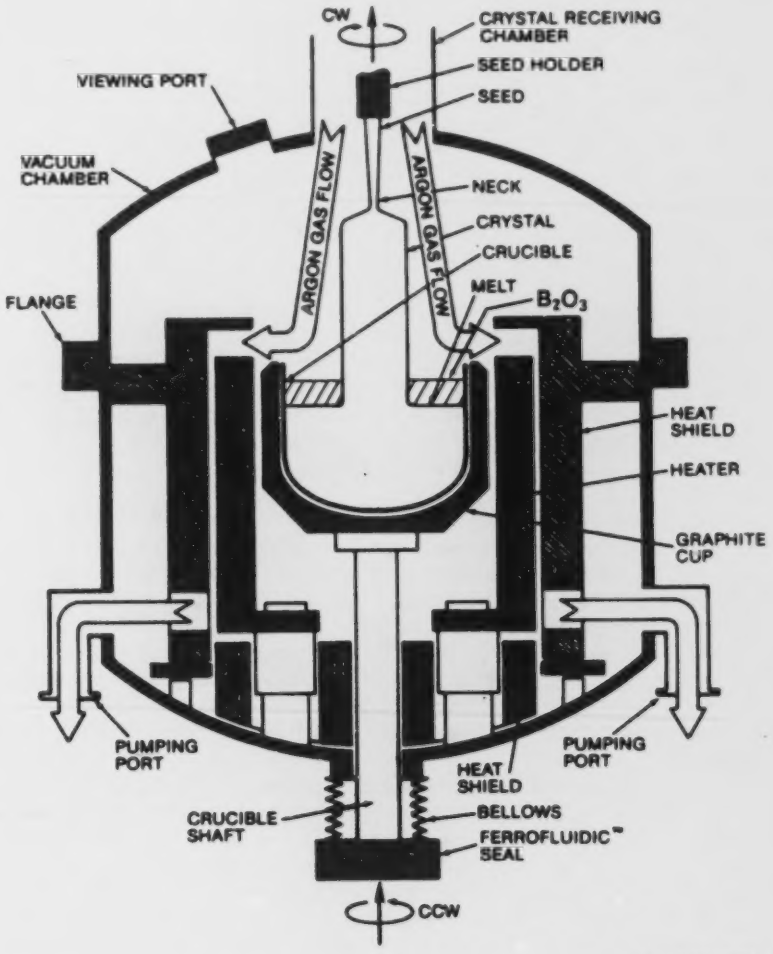
(e) *Monitoring and control of melt stoichiometry.* The stoichiometry of the GaAs melt is recognized to have a pronounced effect on the electrical properties of the grown material. As yet there exists no reliable means to ascertain the stoichiometry of encapsulated melts or to monitor its change with continuing growth. It is strongly recommended that this problem be given high priority.

(f) *Automatic diameter control.* Presently used means for automatic diameter control appear unsuitable for computer-operated seeding, shouldering, and constant-diameter growth. Process automation with diameter control at minimum perturbation of growth and segregation should be pursued, and alternatives to the weighing technique should be studied.

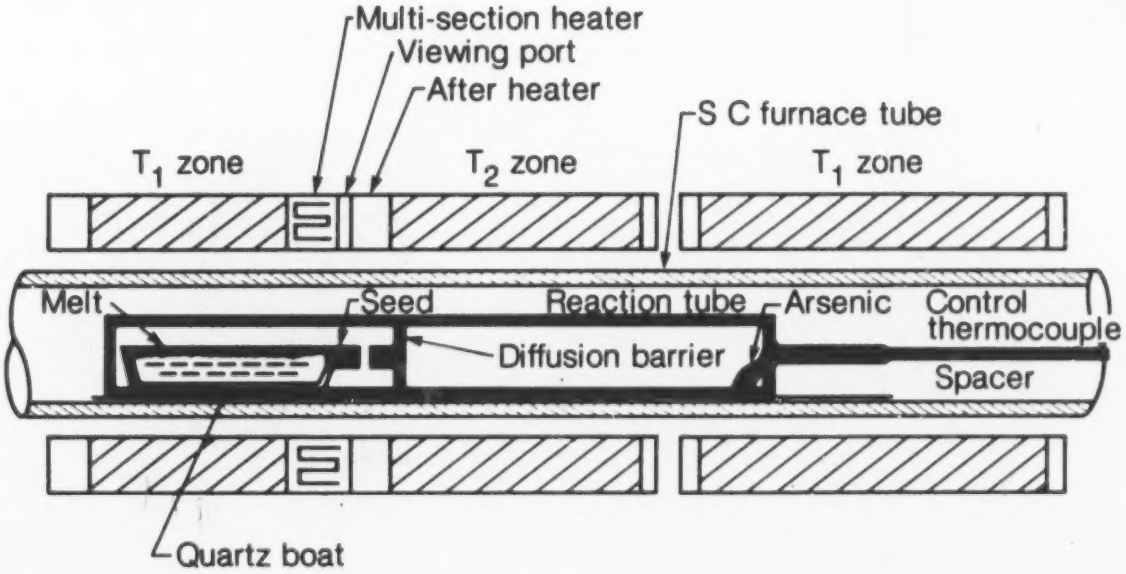
The working group offered many additional suggestions for research activities, such as: exploring in detail the GaAs phase diagram; examining the origin of specified impurities in the melt; determining relevant physical properties; developing high-resolution etching procedures; studying the mechanisms associated with deformation during growth; identifying primary defects affecting the yield of device wafers; and many more. It is the consensus of the group, however, that this research program, being directed *primarily* toward projected materials needs, will develop best if given adequate freedom to pursue emerging problems and that the "burden" of excessive recommendations will probably be an impediment to inventiveness and progress.

It should be noted that the specified goals of the Electronic Materials Group within CAM, as formulated on page 16 of the report of the Industry Participation Workshop

(PUB-5101), were unanimously endorsed by the participants in the workshops, and the members from the industrial community expressed their willingness to participate to the extent possible in the evolving research endeavors.



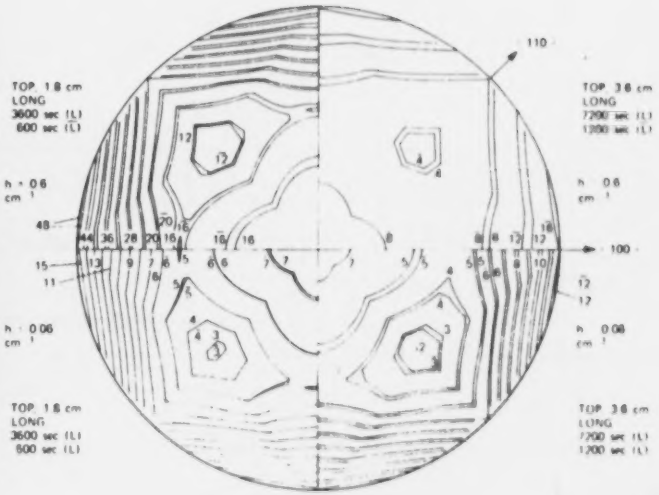
Schematic of a state-of-the-art Czochralski crystal puller. The Czochralski method has the advantage that it can be used to grow much larger crystals for commercial applications. However, at this time there is no commercial method to grow crystals larger than 3 in. in diameter without a prohibitive density of dislocations. Our research will focus in part on improving the method to eliminate the dislocations. (Courtesy of Ferrofluidics Corp.)



Schematic of a horizontal Bridgman furnace for GaAs growth. At present much of the commercially available GaAs is produced by this technique. Major difficulties in using this method are concerned with the control of the stoichiometry of the melt, the non-cylindrical shape of the crystal produced, and the smaller size of the crystal when compared with those obtained with the Czochralski-growth. We will also investigate the use of this method.

(a)

(b)



At present GaAs crystals grown by the Czochralski pulling technique exhibit rather high-dislocation densities for boules of dimensions between 3–4 in. in diameter. These dislocations are one of the major technical problems in the commercial use of GaAs. Dr. Andrew Jordan has proposed that these dislocations are caused by thermal stresses in the boule. A comparison between experimental and analytical results qualitatively confirm this theory. (a) shows experimental results on dislocation distribution. (b) shows analytical stress patterns due to thermal stresses. One of the major efforts in our research will be to quantify the stresses during the crystal growth process and to identify methods for reducing the stresses and eliminating the dislocation. (Courtesy of A. Jordan, Bell Labs.)

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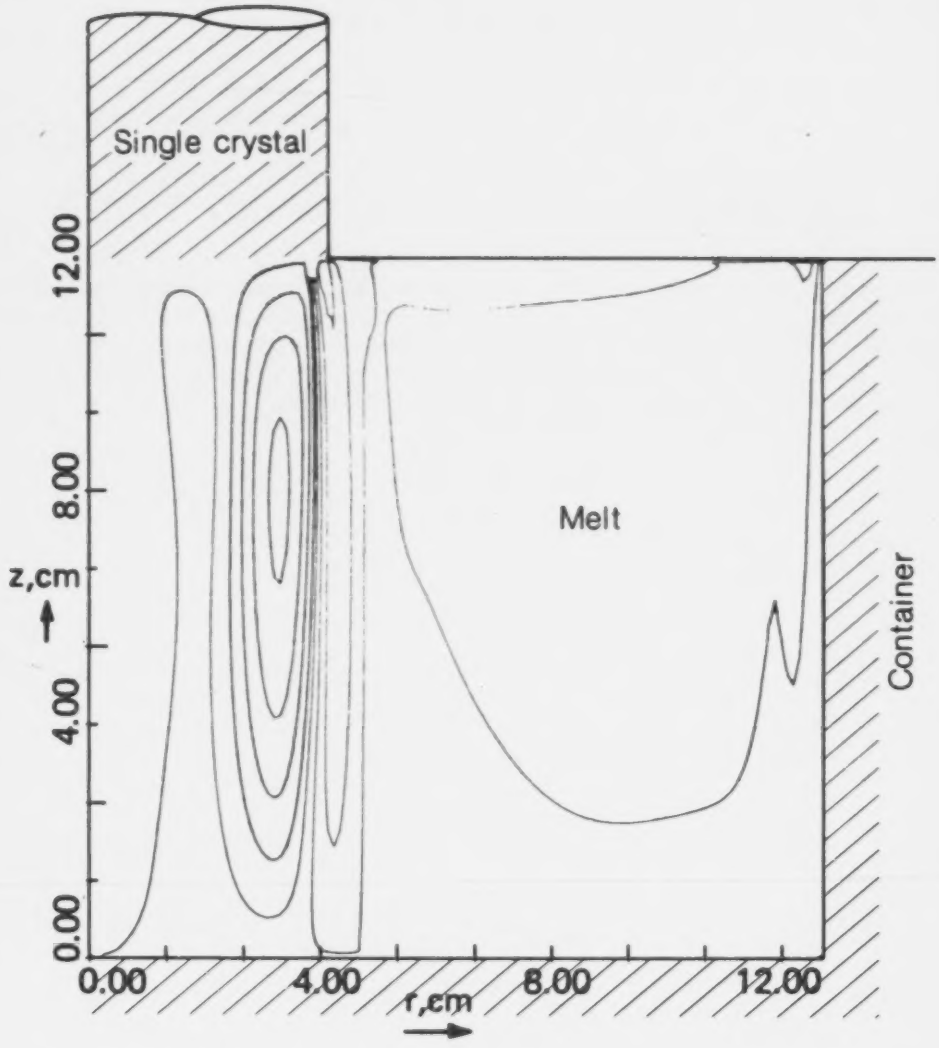

Computer-generated streamlines in the melt during bulk crystal growth of Si in the Czochralski crystal pulling method. These results that were obtained using the numerical finite difference method indicate the complexity of the liquid flow patterns in the melt due to forced convection (rotation), natural convection (density gradients caused by temperature gradients), and magnetic fields. These flow patterns will ultimately affect the quality of the crystal. The complete analysis of flow patterns in gallium arsenide has so far not been attempted. Additional difficulties exist due to the liquid boric oxide encapsulant. (Courtesy of W. Langlois, IBM, San Jose)

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Thin Films and Interfaces

Jerry Woodall (IBM Yorktown), Group Leader
Shyh Wang (LBL and UC Berkeley), Scientific Secretary

Invited Speakers

- D. Collins (Hewlett-Packard): "MBE Growth Technology of III-V Compound Semiconductors"
- M.L. Cohen (LBL and UC Berkeley): "Electronic Structure of GaAs Interfaces"
- J. Freeouf (IBM Yorktown): "Chemical and Electronic Properties of GaAs Surfaces and Interfaces"
- W.D. Laidig (U. of North Carolina): "The Optical and Electrical Properties and the Thermal Stability of GaAlAs/GaAs Interfaces"
- J.R. Shealy (Cornell): "Low-Pressure MOCVD"

Of all the aspects of GaAs device technology, none is more important than thin films and interfaces. The successful fabrication of optoelectronic devices depends critically on the ability to deposit epitaxial semiconductor films with *minority*-carrier properties that approach theoretical limits. This requires that the material contain low densities of unwanted optically and electrically active point and line defects, as well as low densities of unwanted deep-level impurities. Also, the surfaces and interfaces of such devices should be free of states that lead to high recombination velocities.

These requirements hold, for different reasons, for both majority- and minority-carrier high-speed devices. Film quality is critical to the successful fabrication of high-performance metal semiconductor field-effect transistor (MESFET) and modulation-doped field-effect transistor (MODFET) circuits. Even more critical are the electronic properties of the surfaces and interfaces used to fabricate ohmic and Schottky barrier contacts.

Current Status

Within the framework outlined above, we have explored the current status of five topics related to thin films and interfaces, described briefly in the following five sections.

Electronic Structure of GaAs Interfaces

The Berkeley group presented convincing evidence that recent advances in solid-state theoretical physics have resulted in remarkable successes in predicting both the bulk and surface electronic structure of GaAs, particularly the (110) surface. In addition, static structural properties such as lattice constant, cohesive energy, and bulk modulus can be predicted with good accuracy, using as input only the atomic number, atomic mass, and a finite number of crystal structures.

A noteworthy example of this theoretical advance is the good agreement between experimental and calculated values of the band-edge discontinuities for the AlAs/GaAs system. Within the next few years, these methods may be extended to more technologically relevant interfaces, such as disordered Schottky barriers, and may include the effects both of defects and of metal/semiconductor atomic structure. The time is right to begin design of GaAs metallization experiments that can be accurately modeled with these theoretical tools. Examples might include the Al/AlAs or As/GaAs interfaces.

Low-Pressure Organometallic Vapor-Phase Epitaxy

A rather detailed description was presented by the Cornell University group on the growth and characterization of GaAs/AlGaAs structures by organometallic vapor-phase epitaxy (OMVPE). Except for the MODFET and the heterojunction bipolar devices, OMVPE seems to be on a par with molecular beam epitaxy (MBE). Currently there is a problem in forming abrupt GaAs/GaAlAs interfaces, resulting in lower-than-expected mobilities for MODFET structures. It is not certain what causes this problem. Gettering techniques using a liquid metal mixture of Ga-In-Al for arsine have resulted in greatly improved GaAlAs layers, as determined by photoluminescence (PL), at growth temperatures as low as 700°C. These results suggest that gas purity, rather than surface mobility of the adsorbed species, is critical to the layer quality. The V/III gas ratio is critical for layer quality as measured by PL, carrier mobility, conductivity type, and carbon PL intensity.

Common residual impurities in high-purity GaAs layers are Si and Ge. The quality of substrates affects the quality of the epilayers. Semi-insulating Cr-doped GaAs shows the greatest detrimental effects, and when it is etched *in situ* with HCl, the accumulation of Mn is observed. The best films are grown on liquid-phase epitaxy (LPE) substrates.

Molecular Beam Epitaxy

Recent studies on MBE have revealed new information concerning both the so-called DX center and the formation of the oval defect. The Hewlett-Packard group has found, by very careful experimental procedures, that the previously identified DX center may in fact be only one natural dopant donor level associated with the Al composition near the direct-indirect crossover point, with an energy level 150–200 meV below the conduction band. Work at MIT Lincoln Laboratories and IBM has shown that oval defects form by As saturation of Ga drops on GaAs surfaces during MBE growth. The Ga drops form by the nucleation and growth of Ga clusters on gallium oxide precipitates. The precipitates form by disproportionation of gallium suboxide emitted by the Ga effusion cell. Mg doping was found to eliminate the formation of oval defects.

Chemical and Electrical Properties of GaAs Surfaces and Interfaces

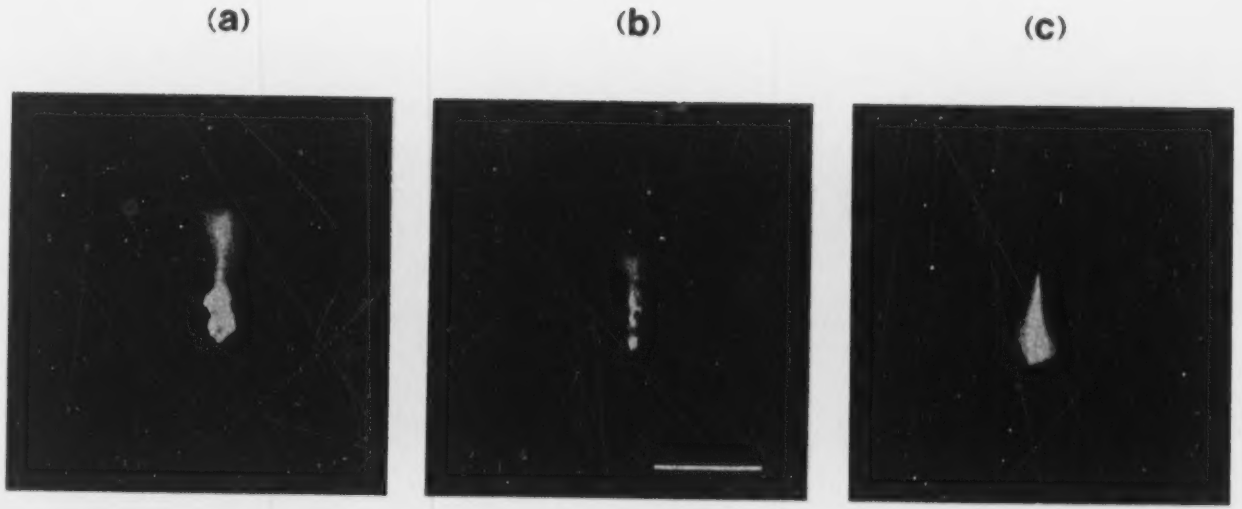
A discussion of the chemical and electrical properties of GaAs surfaces and interfaces revealed that, despite years of research on surfaces and interfaces, we still do not understand the mechanism of Schottky barrier formation in GaAs. For example, the electronic nature of the Au-Ge-Ni ohmic contact is not understood, and currently non-alloyed tunneling n^+ contacts are marginal as ohmic contacts to high-speed devices, owing to the 0.8 V barrier and to a doping saturation at 10^{19} cm^{-3}. In addition, contacts to p-type regions of devices such as laser and heterojunction bipolar devices are not understood and will require improvements for high-speed applications. Fermi-level pinning at GaAs surfaces limits the range of Schottky barrier height. For fabricating devices, industry is still using 20-year-old processing art forms that are not understood. This is clearly a fertile area for research.

Thermal Stability of GaAs/GaAlAs Interfaces

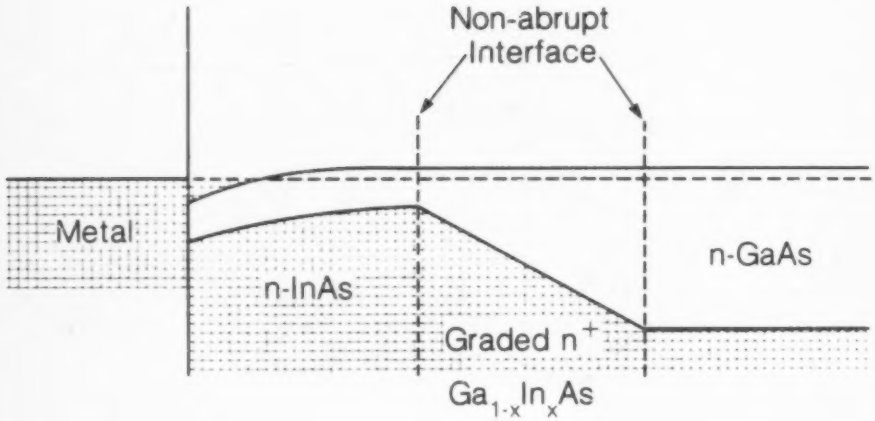
Recent work on annealing GaAs/GaAlAs junctions in the presence of diffusing dopants such as Zn shows that these interfaces, which were once thought to be thermally stable, are in fact very mobile. There are important implications of this finding for the processing of MODFET-type devices.

Summary

We find that much technological progress has been made on the epitaxial growth of high-quality thin films of GaAs and related materials. For MBE, further work is needed to reduce surface defects, such as oval defects, so that medium-scale and large-scale integration can be done on this material. For OMVPE, the mechanism leading to the growth of non-abrupt heterojunctions needs to be understood. For GaAs surfaces and interfaces, little progress has been made on either the technology or science of ohmic or Schottky contacts. We recommend that CAM seriously consider entering the field of "processing science" in an attempt to bridge the gap between fundamental ultrahigh-vacuum surface science and applied processing technology.



SEM picture of typical oval defects observed in an ~ 5 μm thick MBE-GaAs film. The mechanism of formation of these defects is not yet understood; a current model due to Calawa involves a Ga droplet leading to the faceted growth shown in the center of the defect in (a) which, after consumption of the Ga, is then overgrown, resulting in the structure shown in (c). (Courtesy of T. Yamashita and D. Collins, Hewlett-Packard Labs.)



Novel scheme for ohmic contact formation on n-GaAs as proposed by J. Woodall, IBM, Yorktown Heights. The graded transition region from the large gap semiconductor (n-GaAs) to a narrower band gap material (n-InAs) eliminates the barriers between the two materials. This scheme could be of importance to future GaAs IC technology.

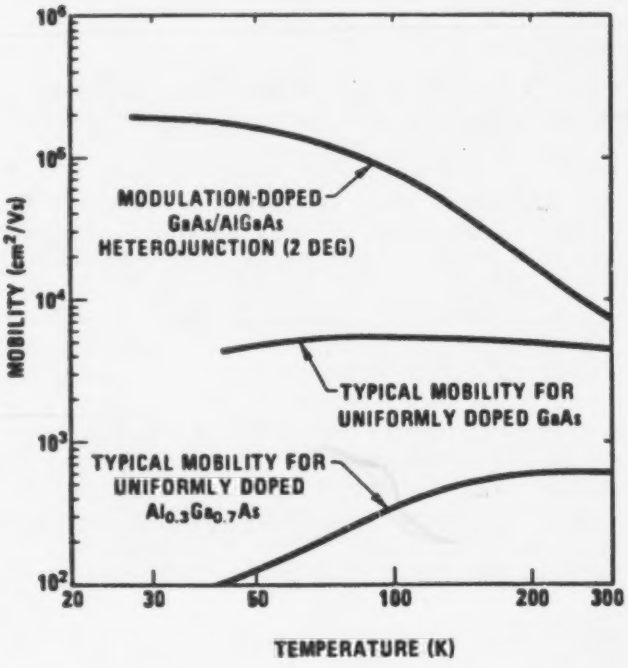


Figure shows the drastic increase of the electron mobility in modulation-doped structures due to the formation of a two-dimensional electron gas (2 DEG).

Characterization

Pierre M. Petroff (Bell Labs, Murray Hill), Group Leader
Eicke R. Weber (LBL and UC Berkeley), Scientific Secretary

Invited Speakers

- D. Collins (Hewlett-Packard): "Problems of Substrate Defects/Epilayer Relationships"
- C. Evans (Evans & Associates): "SIMS and Auger Spectroscopy of GaAs"
- R. Gronsky (LBL and UC Berkeley): "The New Atomic Resolution Microscope in Berkeley"
- A. Hunter (Hughes): "Impurity and Deep Defect Distribution in Semi-Insulating GaAs"
- J. Jaklevic (LBL): "Heavy-Ion RBS of Implanted Layers and Interfaces of GaAs"
- L.A. Ledebo (U. of Lund, Sweden): "Transition-Metal Impurities in GaAs and Their Influence on Devices"
- J. Merz (UC Santa Barbara): "Luminescence of GaAs and Related Compounds"
- F. Pollak (Brooklyn College): "The Study of Defects in GaAs by Raman Spectroscopy"
- F. Ponce (Hewlett-Packard): "The Structure of Defects in GaAs"
- D.C. Reynolds (AFAL, Wright Patterson): "High-Resolution Spectroscopy for Shallow Levels in GaAs"
- R. Sinclair (Stanford): "High-Resolution Electron Microscopy of Semiconductor Interfaces and Defects"

The goal of this workshop was to select a number of *relevant* and *fundamental* problems associated with the growth of GaAs crystals and their subsequent processing. The characterization techniques suitable for tackling these problems were discussed extensively. This section summarizes the highlights of this working group session and makes specific recommendations for future work in this CAM program.

Problems with GaAs and Related Compounds

It became evident from a number of the contributions that our knowledge of the basic properties (electronic and atomic configuration) of many defects is limited. The nature of the EL2 center, the DX center, and other deep-level defects was discussed at length.

We also noted a complete absence of new data on the elementary point defects in GaAs. In our opinion, the severe lack of knowledge concerning the V_{Ga}, V_{As}, I_{Ga}, and I_{As} defects is hindering our understanding of the complex and important defects, such as EL2 and DX centers. We recommend that basic experiments involving electron irradiation and sophisticated spectroscopic techniques be addressed to this problem.

The EL2 Center

The origin of the EL2 center is still unclear. It is well established, however, that its concentration is tied to the As/Ga ratio during crystal growth (i.e., it is associated with the material stoichiometry). The results of electron paramagnetic resonance (EPR) investigations allow the conclusion that the anion antisite defect is at least part of the EL2 center. Besides appearing in as-grown undoped bulk GaAs, this defect has been detected by EPR in neutron- and electron-irradiated and plastically deformed GaAs.

These observations, together with the results of annealing experiments, have led to the conclusion that there exists a "family" of EL2 centers. Evidence in support of this conclusion comes from the various energy levels that have been reported for this defect. Even after 10 years of data collection, there remains a raging controversy centered on the nature of the defect. It is not yet clear whether EL2 is an isolated intrinsic defect, a complex of the form $As_{Ga} - V_{As}$ or $As_{Ga} - V_{Ga}$, or, in some cases, an oxygen-associated defect, or even a more complex defect.

Several questions associated with the effects of EL2 on the electronic properties of the material remain to be clarified, notably:

1) Is EL2 responsible for the Fermi-level pinning of the Schottky barriers in GaAs?
2) Is EL2 related to another donor level?
3) What is the compensation mechanism involving EL2 that makes possible the growth of semi-insulating GaAs?
4) What other impurity levels are involved in the compensation mechanism? Specifically, what is the role of carbon and transition metals in GaAs?

Antisite Defects

Knowledge of the anion antisite defects has progressed rapidly over the last few years, thanks to the EPR and optically detected magnetic resonance (ODMR) results for GaP and GaAs. For GaAs, however, the question of the existence of an $As_{Ga} - V_{Ga}$ complex and of other complexes is still open because of the large line widths in the EPR spectra. Electron

nuclear double resonance (ENDOR) experiments might answer this question in the near future. The new magnetic circular dichroic absorption ODMR technique, the first successful results of which were reported during the workshop, offers further information on the nature of antisite defects.

We should also note that little is known about the Ga_{As} antisite defect. Is this defect associated with the A and B hole traps, or is it connected with the shallow acceptor levels (E_v + 78 meV, E_v + 200 meV) detected in bulk GaAs?

The DX Center

The second major class of defect, the DX center, needs further investigation. Much work has been done on this problem since it was suspected that the DX center played a role in the degradation of light-emitting devices. There is evidence that the DX level is important for the electronic properties of n-type Al_{1-x} Ga_xAs ($x > 0.25$). It is known that the DX complex involves a donor impurity (D) and perhaps another unknown defect (X). It has been observed in $Al_xGa_{1-x}As$ ($x > 0.25$) and $GaAs_{1-x}P_x$ ($x > 0.3$) doped with a large variety of donor species.

Investigations of the band-structure effects on the DX center have shown that its level ($E_c - 0.35$ eV) is tied to the X point of the conduction band. The most important questions concerning the nature of the defect are:

1) Is it a simple donor defect whose level is tied to the conduction-band minimum or the X points for $x \geq 0.22$? The suggestion was made by Ledebo that an alternative explanation for the various anomalous effects in the semiconductor alloys is simply the deepening of the otherwise hydrogenic donors as soon as the L-band comes close to the conduction-band edge. This may cause "deepening" of shallow donor levels in $Al_xGa_{1-x}As$ ($x \gtrsim 0.3$) and in $GaAs_{1-x}P_x$ ($x \gtrsim 0.3$).
2) Is it a donor-impurity complex, or a donor-point defect complex? For example, the V_{As} has been mentioned as the "X" part of the defect, but this has not been convincingly established.

Because of their technological importance to devices, we recommend further basic studies on both the EL2 and DX centers. These studies could, for example, examine the role of amphoteric and other impurities, of annealing, and of stoichiometry variations, using bulk and epitaxial GaAs of high purity.

Dislocations

The workshop did not produce any new insight on the structural or electronic properties of dislocations. The questions of the atomic arrangement of the core of the α and β dislocations, including the glide- and shuffle-set configurations, remain to be solved. The electrical activity of dislocations and their energy levels should be studied because of their importance in device degradation.

The dynamics of dislocation motions—including studies of critical shear stress at high temperature and for various dopants and dopant concentrations—appears to be important for good control of bulk GaAs crystal growth. In the same context, the effects of substrate dislocations and other structural defects on the quality of the epitaxial layers, or on the performance of devices, still need further study.

Dislocation-point defect interactions, which have been shown to be important in the degradation processes, will also be an important issue in achieving higher-quality, defect-

free bulk GaAs.

Questions of defect control, such as gettering effects and the determination of the stoichiometry of GaAs crystals, are technologically important but were not discussed by the group. They deserve special attention in the future.

Characterization Techniques

A large part of this group's session was devoted to the characterization techniques that are necessary for this type of investigation. These were classified in the two categories: structural characterization and electronic characterization and are listed at the end of this section.

Structural Characterization

The imaging methods deal primarily with extended defects (dislocations, stacking faults, and precipitates). Ideally, high-resolution transmission electron microscopy (TEM) must be supplemented by microscopic analytical work on problems of crystal growth and device applications. To this end, small-electron-probe scanning transmission electron microscopy (STEM) and TEM techniques such as electron energy-loss spectroscopy (EELS) and energy-dispersive spectroscopy (EDS) are essential.

It was clearly stated (Sinclair) that ultrahigh-resolution TEM will require more careful and extensive image computation than conventional high-resolution TEM as it becomes a more widespread technique. The type of problems that could be treated more easily by ultrahigh-resolution TEM needs to be defined in the field of semiconductor defects. However, it can be expected that this technique will be most important for chemical identification, applications to the study of nucleation and growth of microprecipitates (10 Å), and the distribution and morphology of pre-precipitation clusters.

Other structural techniques—such as x-ray topography for studying the dynamics of crystal growth and defect generation, and heavy-ion Rutherford backscattering (RBS) for studying substitutional impurities—will be of great use to the CAM GaAs crystal-growth effort.

Chemical analytical techniques with ultrahigh sensitivity will probably be essential to this program, for the purposes of which, secondary-ion mass spectroscopy (SIMS) appears to be the best prospect. However, other techniques, such as particle activation analysis and other accelerator-related techniques, could be developed and, presumably, proved useful.

Electronic Characterization

Spectroscopic techniques useful for the GaAs defect problems have already been developed for defect studies of Si and ionic crystals. Their sensitivity and resolution are well established. To attack the problems mentioned in this report, it is recommended to use a combination of spectroscopic techniques, with emphasis on making them quantitative as well as qualitative—e.g., EPR, photoluminescence, and infrared absorption, as well as recently developed techniques such as photoacoustic and photothermal spectroscopy, Raman scattering, photothermal ionization spectroscopy, and picosecond spectroscopy. The testing of simple device structures should complement these spectroscopic techniques.

Spatially Resolved Spectroscopic Techniques

These would combine the advantages of microscopic structural and spectroscopic techniques. They have been listed at the end of this section, under "Electronic Characterization, Defect-Mapping Techniques." All are based on small-probe scanning instruments and yield not only mapping information but also, in conjunction with other techniques, structural information via STEM and chemical information via EELS and EDS. Because of their power and versatility, their importance to the CAM Electronic Materials Program cannot be overemphasized.

Conclusions

The consensus of the group was that the characterization and crystal-growth research efforts at CAM should be intimately linked, with rapid and open communications. This will be essential for the success of this program. The many problems associated with crystal growth will require a major characterization effort involving not only university and LBL participation but also industrial cooperation.

We would like to stress that the problems raised in this report are not presently prime targets of industrial research. They are, however, perfectly suited for long-term basic research because of their relevance and fundamental character.

Finally, the high level and abundance of sophisticated characterization techniques available on site suggest the following question: Should this part of CAM have a broader goal than crystal growth? For example, should we also use the facility for other materials-related problems, e.g., processing science, very small-device materials science, and micrometallurgy?

Characterization Techniques Recommended for the CAM Electronic Materials Program

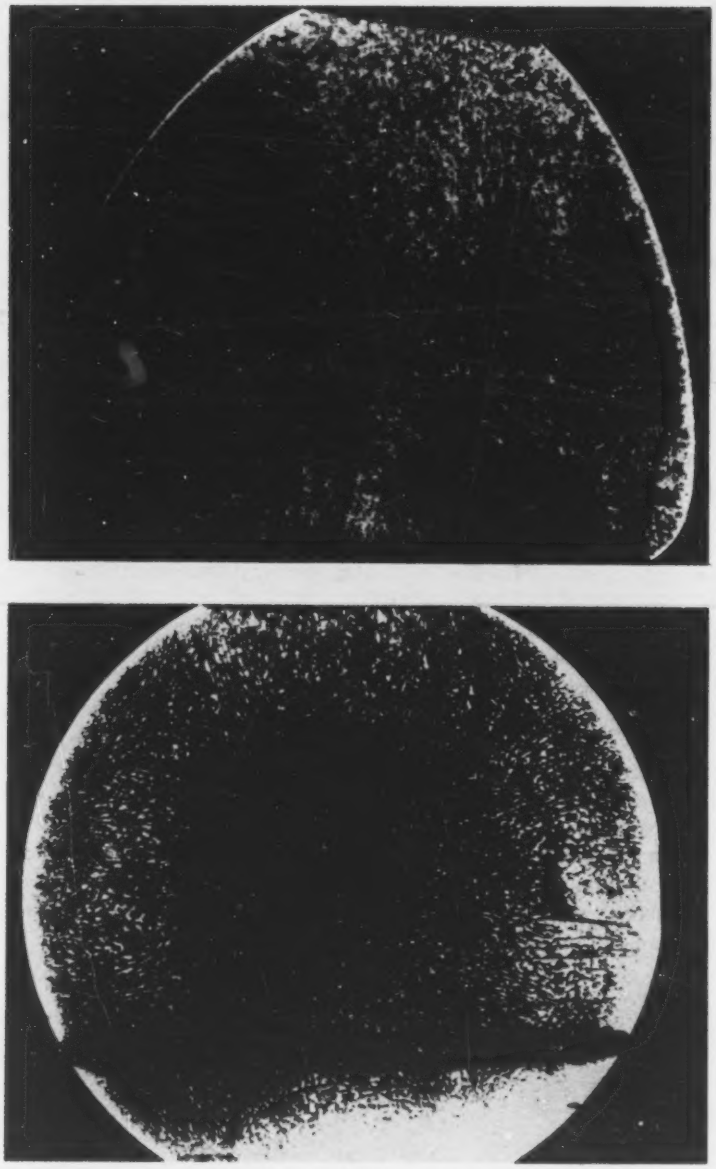
Structural Characterization

- Chemical etching techniques
- Electron microscopy
  - — Standard transmission electron microscopy, including high-resolution electron microscopy and analytical electron microscopy (e.g., electron energy-loss spectroscopy)
  - — High-Voltage Electron Microscope
  - — Atomic Resolution Microscope
- X-ray topography
  - — With standard sources, including rotating anode
  - — Using synchrotron radiation
- Beam techniques
  - — Neutron and particle activation analysis
  - — Heavy-ion Rutherford backscattering

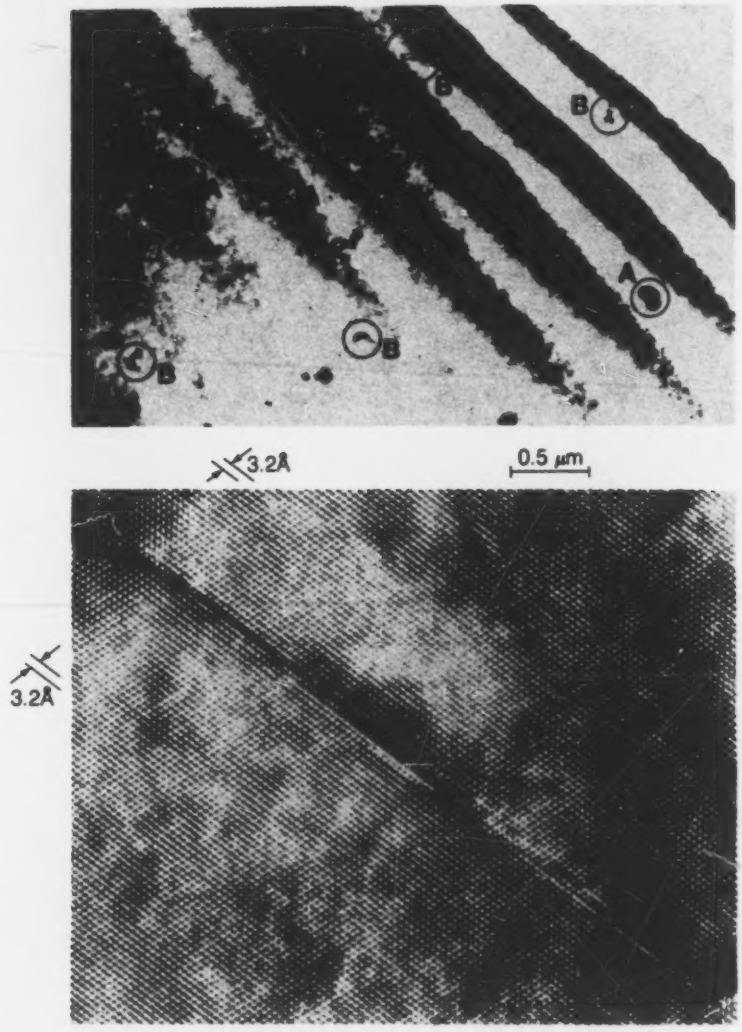
  - — Auger spectroscopy/microscopy
  - — Secondary-ion mass spectroscopy (SIMS), including accelerator-supported SIMS
- Photoacoustic and photothermal microscopy

Electronic Characterization

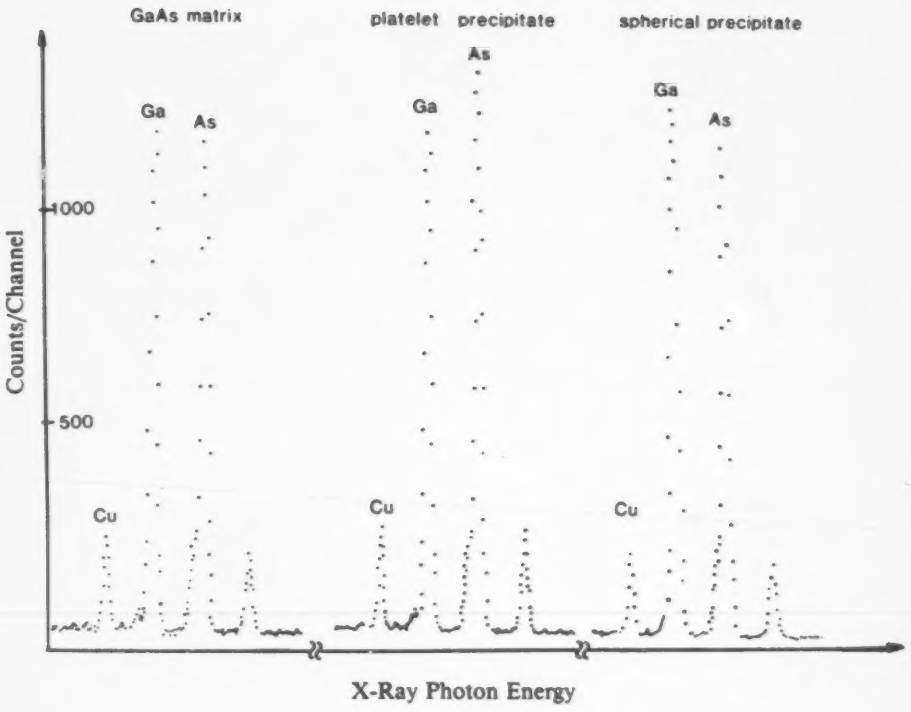
- Electrical resistivity, carrier concentration
  - — Four-point probe, etc.
  - — Hall effect
- Junction-transient techniques
  - — Standard deep-level transient spectroscopy (DLTS)
  - — Optically excited DLTS, optical transient-capacitance spectroscopy, photocapacitance
- Paramagnetic resonance
  - — Standard electron paramagnetic resonance (EPR)
  - — Photo-excited EPR
  - — Optically detected magnetic resonance
- Optical absorption
  - — High-resolution near- and far-infrared spectroscopy
  - — Near-bandgap absorption
- Photoluminescence with photoluminescence excitation spectroscopy (including optically detected magnetic resonance)
- Defect-mapping techniques
  - — Optical absorption (especially near-bandgap absorption)
  - — Photoluminescence
  - — Cathodoluminescence
  - — Deep-level transient spectroscopy
  - — Electron-beam-induced current
- Recently developed techniques
  - — Photoacoustic and photothermal spectroscopy
  - — Raman scattering
  - — Photothermal ionization spectroscopy
  - — Picosecond spectroscopy
  - — Scanning tunneling microscopy



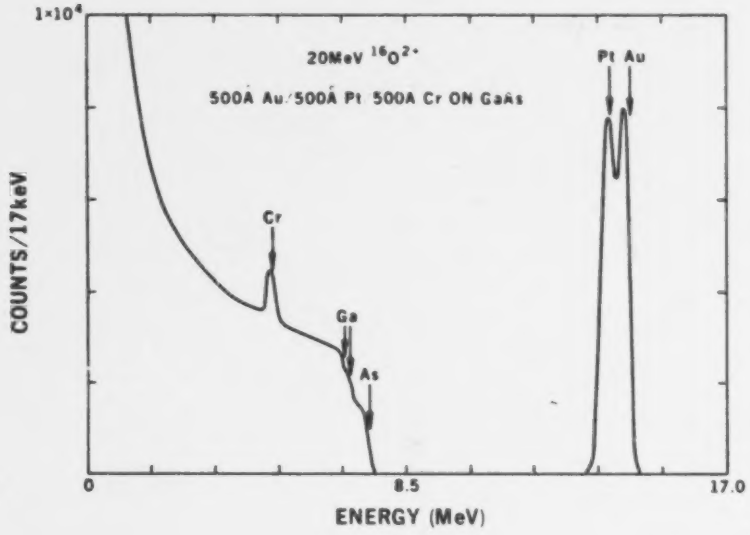
X-ray topographs showing the dislocation in state-of-the-art semi-insulating GaAs single crystals: (a) Cr-doped HB crystal and (b) undoped LEC crystal. For certain applications these dislocation densities prevent acceptable device yield. (Courtesy of M. Scott, Hewlett-Packard Labs.)

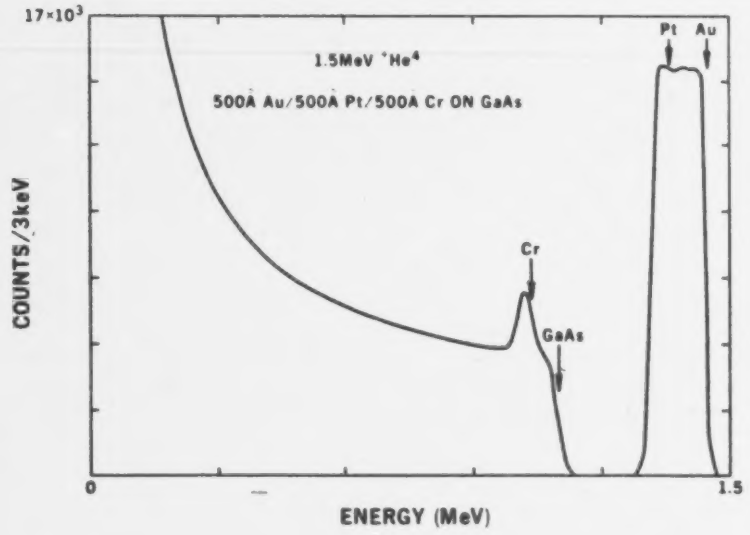


(a) Electron microscope overview photograph of defects in p-GaAs (8×10^{18} Zn/cm^3) used as substrate for AlGaAs light-emitting diodes. A: spherical precipitates; B: platelet precipitates. (b) High-resolution "lattice image" of a platelet precipitate (type "B"). Results of analytical microscopy of these defects are shown in the following figure. (Courtesy of Z. Liliental, Arizona State U.)



Energy dispersive x-ray spectra (EDX) of GaAs matrix and two different types of precipitates. Figure shows only parts of the spectra, containing Ga and As lines (Cu lines are from the specimen grid). The intensity ratio of the Ga and As lines is different, indicating different stoichiometry of the defects. Such data, when combined with information from electron energy loss spectroscopy (EELS) and the analysis of high-resolution electron microscopy images, allow the identification of the composition of the defects. As an example, the As-rich platelet precipitates were identified to be $ZnAs_2$. (Courtesy of Z. Liliental, Arizona State U.)





Comparison of heavy ion (HI) and helium Rutherford backscattering spectra (RBS) of the same metal-GaAs structure used for Schottky contact formation. The enhanced mass resolution in the HIRBS spectrum is clearly noticeable.

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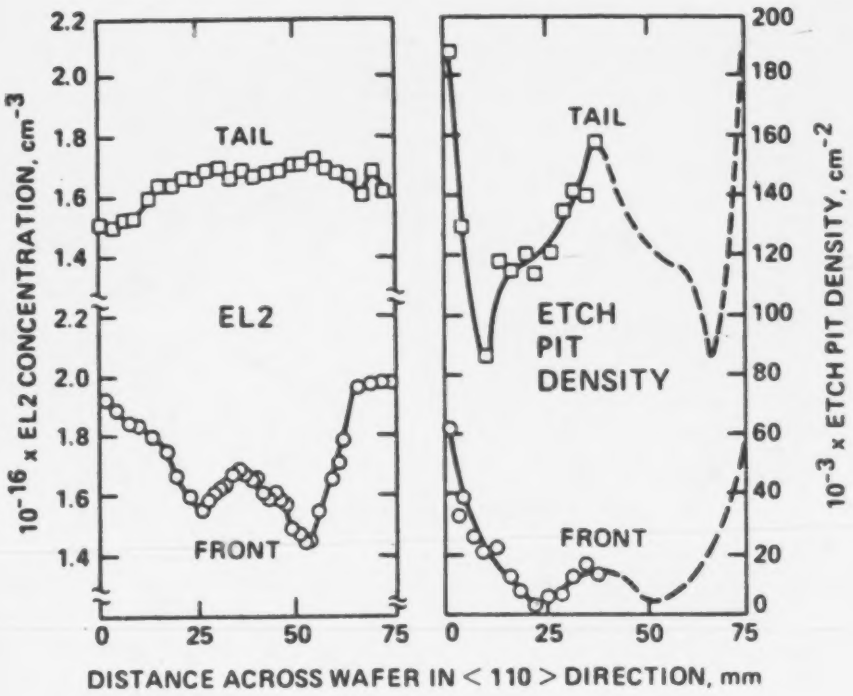
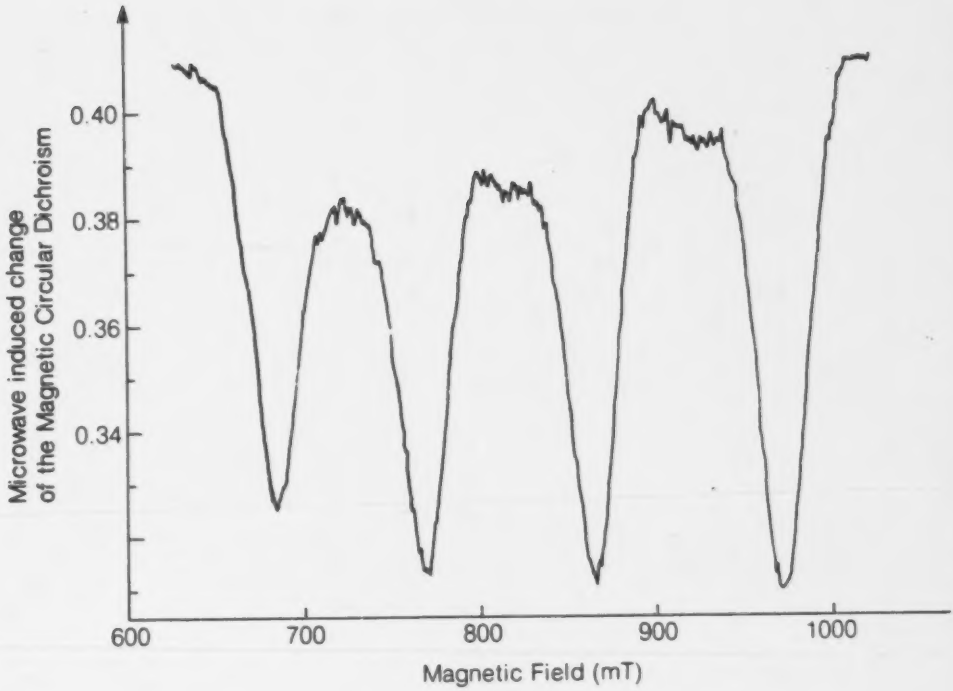


"EL2"-concentration and etch pit density across a 3-in. diameter LEC GaAs crystal grown from near stoichiometric melt. Obviously, dislocations are not the only source of EL2 formation; in addition, stoichiometry fluctuations on a microscale may lead to EL2 defect creation. [After D.E. Holmes *et al.*, Appl. Phys. Lett. 42, 419 (1983)]



Optically detected magnetic resonance signal of the As_{Ga} antisite defects in GaAs as presented for the first time during the workshop. (Courtesy of B.K. Meyer, J.M. Spaeth, and M. Scheffler, University of Paderborn, W. Germany)

ELECTRONIC MATERIALS WORKSHOP AGENDA

	MONDAY 10/10		TUESDAY 10/11		WEDNESDAY 10/12
9:00	REGISTRATION: Bldg. 50 Auditorium Lobby	8:30	APPLICATIONS (Joint Session) *Group Leader/Secretary* R. Bauer /N. Amer	9:00	DISCUSSION OF DRAFT REPORTS WITH GROUP AND REVISIONS
10:00	WELCOME K. Pitzer, NCAM Director	10:15	COFFEE BREAK		
10:20	INTRODUCTION TO WORKSHOP E. Haller	10:30	CHARACTERIZATION, THIN FILMS, BULK CRYSTAL GROWTH (Joint Session)		
10:45	PLENARY TALK: J. Blakemore *(Physics of III-V Compounds)**	11:30	LUNCH: LBL Cafeteria	11:30	LUNCH: LBL Cafeteria
11:30	LUNCH: LBL Cafeteria	12:30	THIN FILMS AND INTERFACES *Group Leader/Secretary* J. Woodall /S. Wang	1:00	REPORTS OF GROUP LEADERS TO THE WORKSHOP
1:00	PLENARY TALKS: R. Burmeister *(GaAs-based Devices)**		CHARACTERIZATION *Group Leader/Secretary* P. Petroff /E. Weber	2:30	CLOSING REMARKS
	J. Carruthers *(GaAs Bulk Crystal Growth)**		BULK CRYSTAL GROWTH *Group Leader/Secretary* A. Witt /B. Rubinsky	3:00	END OF WORKSHOP
2:45	COFFEE BREAK				
3:15	M. Panish *(Compound Semiconductor Epitaxy)**				
	J. Schneider *(Defects in GaAs)**				
5:00	WINE TASTING LBL Cafeteria				

* Topic of Talk, precise title will be announced later

ELECTRONIC MATERIALS WORKSHOP AGENDA

	TUESDAY, 10/11, DETAIL
8:30	APPLICATIONS (Joint Session)
	- R. Burnham "Multiquantum Well Lasers by MOCVD"
	- R. Eden "Applications and Materials Implications for Commercial GaAs ICs"
	- L. Eastman "Compound Semiconductor Materials for High Speed Applications"
10:15	COFFEE BREAK
10:30	CHARACTERIZATION, THIN FILMS, BULK CRYSTAL GROWTH (Joint Session)
	- D. Collins "MBE Growth Technology of III - V Compound Semiconductors"
11:30	LUNCH
12:30	THIN FILMS AND INTERFACES:
	- M. L. Cohen "Electronic Structure of GaAs Interfaces"
	- J.R. Shealy "Low Pressure MOCVD"
	- J. Freeouf "Chemical and Electronic Properties of GaAs Surfaces and Interfaces"
	- W. D. Laidig "The Optical and Electrical Properties and the Thermal Stability of GaAlAs/GaAs Interfaces"
	CHARACTERIZATION: (See next page for details)
	• Electrical Characterization - A. Hunter, L.A. Ledebo
	• Optical Characterization - J. Merz, D.C. Reynolds, F. Pollak
	• Structural Characterization - R. Sinclair, F. Ponce, R. Gronsky
	• Beam Techniques - C. Evans, J.Jaklevic
	BULK CRYSTAL GROWTH:
	- A. Jordan "Defect Formation due to Thermal Stresses in LEC Growth of GaAs"
	- W. Langlois "Fluid Dynamics in LEC Growth"
	- D. Miller "Low Pressure LEC Growth of GaAs"
	- D.L. Barrett "High Pressure LEC Growth
	- J. Vaughan "Bridgeman Growth of GaAs"

CHARACTERIZATION SESSION AGENDA

	TUESDAY 10/11
10:30	**Joint Session:**
	D. Collins: "Problems of substrate defects/epilayer relationships"
11:30	**LUNCH: LBL Cafeteria**
12:30	**Electronic Properties of Defects in GaAs**
	A. Hunter: "Impurity and Deep Defect Distribution in s.i. GaAs"
	L.A. Ledebo: "Transition Metal Impurities in GaAs and their Influence on Devices"
	J Merz: "Luminescence of GaAs and Related Compounds"
	D.C. Reynolds: "High Resolution Spectroscopy for Shallow Levels in GaAs"
	F. Pollak: "The Study of Defects in GaAs by Raman Spectroscopy"
3:00	**COFFEE BREAK**
3:15	**The Structure of Defects in GaAs**
	R. Sinclair: "High Resolution Electron Microscopy of Semiconductor Interfaces and Defects"
	F. Ponce: "The Structure of Defects in GaAs"
	R. Gronsky: "The New Atomic Resolution Microscope in Berkeley"
4:45	**COFFEE BREAK**
5:00	C. Evans: "SIMS and Auger Spectroscopy of GaAs"
	J. Jaklevic: "Heavy Ion RBS of Implanted Layers and Interfaces of GaAs"

NCAM

ELECTRONIC MATERIALS PROGRAM

DISCUSSION DOCUMENT

August 31, 1983

ABSTRACT

An Electronic Materials Program is proposed that will focus on the major scientific problems to be solved before viable very-large-scale integrated circuits based on gallium arsenide crystals can be developed by industry. An interdisciplinary basic research effort, both experimental and theoretical, will be directed at the mechanisms of defect formation and contamination during bulk crystal growth, the relationship between the structure and electronic properties of interfaces, and the effects of substrate defects on the quality of epitaxial thin films.

INTRODUCTION

Recent progress in the design and fabrication of prototype electronic devices based on gallium arsenide (GaAs) crystals has led to a worldwide consensus that the extraordinarily high speed and low power consumption of GaAs devices can be exploited in very-large-scale integrated circuits (VLSI circuits) in the relatively near future. This optimistic view is well justified. Nonetheless, it is clear that GaAs technology does not rest on as firm a scientific foundation as did silicon technology in the 1960s. Not only is there inadequate basic knowledge of the structure and properties of GaAs, there are also a number of serious practical difficulties inherent in the use of compound semiconductors. These include defects related to stoichiometry, such as antisite defects, as well as problems specifically related to GaAs, such as the lack of a stable native oxide, very high surface-state densities, a high arsenic vapor pressure, and a low ductile-brittle transition temperature.

In the past, semi-insulating GaAs crystals were produced by doping, which compensates uncontrolled shallow impurities. In addition, isoelectronic doping (e.g., with Si) was used to provide solution hardening, which results in lower dislocation densities. Yet these crystals are not sufficiently stable during heat treatment (thermal conversion), especially after ion implantation. An apparently more promising compensation mechanism has recently been described for chromium-free GaAs grown by the liquid-encapsulation Czochralski (LEC) method. Here nonstoichiometric defects (As on Ga sites) serve as deep donors, thus compensating shallow acceptors.

It is proposed that a number of the above-stated problems related to GaAs be investigated over the next three to five years, making use of the novel approach to research that will characterize the National Center for Advanced Materials (NCAM). This multidisciplinary facility, which is planned for construction at the Lawrence Berkeley Laboratory, will foster close collaborations between industrial, national laboratory, and university scientists in large, basic research programs focused on problems of national interest.

The proposed program of experimental and theoretical research will focus on two goals:

1. An understanding of the mechanisms of defect formation in GaAs bulk crystals, so as to allow the production of large-diameter (~3 inches), high-purity, semi-insulating crystals with fewer than 10 dislocations/cm^2.

2. Elucidation of the structure and electronic properties of interfaces between GaAs and other semiconductors, as well as insulators, metals, gases, and vacuum.

Concomitant with this research program will be a continuing effort to characterize the bulk and interfacial properties of the GaAs crystals, through both existing and newly developed methods. Throughout, strong consideration will be given to possible applications of GaAs crystals in novel devices.

It is expected that the desired properties of GaAs bulk crystals will be achieved as the program evolves. Close ties with industry will provide the necessary feedback for program adjustments along the way.

SCIENTIFIC PROGRAM

.GaAs BULK CRYSTALS

Compound semiconductors differ fundamentally from elemental ones in that they allow a great multiplicity of defects at the atomic level, contain volatile and corrosive components, and have variable melting points that are functions of the chemical composition. In addition, the removal of unwanted, residual impurities from such materials is much more difficult than it is from elemental substances. The shallow levels produced by such impurities has hitherto required compensation by a deep level. In the past, this compensating level has been introduced with chromium; more recently; with the EL2-antisite defect.

Experimental Studies

The three principal crystal-growth techniques tried thus far – Czochralski, horizontal Bridgman, and vertical Bridgman – have their advantages and disadvantages. Experts in the field have not yet reached a consensus on which of these techniques is the most likely to yield large-diameter, low-defect-density, high-purity, semi-insulating GaAs crystals that can be used as substrates for VLSI circuits.

With the addition of a liquid encapsulant over the melt in furnaces of the conventional Czochralski and Bridgman types, small-diameter Group III-V crystals showing excellent properties have, at times, been produced. Growing large-diameter, high-quality bulk crystals with predictable characteristics, however, requires a much more detailed understanding of the relationships between the growth parameters and the material properties.

The growth parameters include: thermal gradients throughout the melt and the growing crystal; convective mixing of the melt; chemical composition and vapor pressure surrounding the melt and the growing crystal; thermal symmetry; and growth velocity. All of these parameters affect the shape of the crystal/melt interface during the liquid-solid transformation and the incorporation of minor constituents and vacancies at the interface; they thus determine the degree of chemical and structural imperfection. Interactions among point defects during cooling of the crystal may also be responsible for the formation or growth of dislocations, vacancy clusters, vacancy-impurity complexes, and antisite defects. The presence of an encapsulant such as boric oxide may be responsible for defect formation due to compressive stresses applied to the surface of the crystal upon cooling.

In conventional Czochralski and Bridgman furnaces, the growth parameters are strongly coupled. For research purposes, however, it is imperative that they all be independently variable so that their respective effects on the material properties can be identified. Therefore it is proposed to develop special apparatus that will provide for controlled growth of GaAs (and, in the future, other compound semiconductors) and allow the study of defect formation and its effects on the properties of the crystals.

A crystal-growth furnace designed to enable the location and shape of the crystal/melt interface to be controlled will allow studies of the effects of: (1) convective mixing in the melt, both with and without magnetic fields; (2) the vapor pressure over the melt (which controls its stoichiometry); and (3) the cooling process. Control over the location and shape of the crystal/melt interface and over the cooling process can be achieved by incorporating heat pipes in the furnace.

Control of convection in the melt will be complex, owing to a destabilizing thermal gradient, surface flows (driven by surface tensions at the melt/gas or melt/encapsulant interface), and rotation of the seed or the crucible.

Some of the most important unresolved problems associated with the three principal crystal-growth techniques are:

1. Czochralski (as LEC): compressive stress on the crystal due to solidified encapsulant residues; difficulty in controlling the arsenic loss from the crystal during the growth process; difficulty in controlling the diameter of the crystal under conditions of very low thermal gradient.

2. Horizontal Bridgman: difficulty in controlling and modeling the shape of the crystal/melt interface, due to the marked asymmetry around the crystal-growth axis.

3. Vertical Bridgman: difficulty in controlling the stoichiometry at the interface, due to its inaccessibility; impurities from the container; inhomogeneities in the crucible material.

Numerical Modeling

To gain a complete understanding of the crystal-growth process, the events that occur in the crystal, in the melt, and at the interface between them must be modeled. Our ultimate goal is to develop a numerical model that can predict the time-dependent thermophysical phenomena occurring in all three regions. To this end, our experimental efforts will be complemented by numerical simulation of the crystal-growth process, using the "front-tracking" finite element technique and possibly the "vortex" method.

In the liquid region, we will model the fluid flow as a function of the thermal field and its effect on the incorporation of arsenic at the crystal/melt interface. In the solid region, the emphasis will be on modeling the temperature distribution caused by forced or natural convection in the surrounding environment (gas and the liquid encapsulant). The results obtained, combined with those from existing stress models, will provide a better understanding of defect formation during the cooling process.

The front-tracking finite element program will also be used to track continuously the position of the liquid-solid interface and to recognize local instabilities and oscillations in its position, including capillary effects and local thermodynamics. Furthermore, the results obtained by the same program in the liquid and solid regions can now be matched at the interface.

GaAs INTERFACES AND THIN FILMS

Interfaces play a dominant role in the many thin-film growth techniques, as well as in all doping and contacting methods. The term "interface" is used here in its most general sense, namely, as any boundary between an object (here a single crystal of GaAs) and the surrounding medium; it includes the boundaries between GaAs and metals, insulators, semiconductors, liquids, gases, and vacuum. (A special case, the interface between solid and liquid GaAs, was discussed in the preceding section.)

A good understanding of interfaces is necessary for a clear distinction to be drawn between the two sources of structural defects in thin films. One source of defects is due to imperfections in the growth process of the thin film, whereas the other is due to the migration of these defects. It is not clear a priori whether any

given class of defects, such as intrinsic point defects, impurities, impurity clusters, or dislocations, has a detrimental or beneficial effect on the properties of electronic devices. Many defect interactions occur in parallel during the numerous high-temperature cycles that are required in the fabrication of any such device. The study of defect interaction and propagation is essential to the development of quality criteria for GaAs substrates and bulk single crystals.

The initial research program on interfaces and thin films will encompass three major areas: molecular beam epitaxy, ion implantation, and the synthesis of insulating films.

CHARACTERIZATION OF DEFECTS AND INTERFACES

The characterization of semiconductor materials grown under systematically varied conditions is aimed at improving the growth techniques and understanding better the nature and properties of crystal defects. It requires that appropriate analytical methods be available. The characterization part of this program will combine the use of existing, proven methods with a research effort designed to develop new methods for attacking specific problems. Because the scope of such a program is large, it is convenient to divide it in terms of specific problems related to the properties of the bulk crystal and its various interfaces.

Bulk GaAs – Structure of Defects

The microscopic structures of most lattice defects in GaAs are not yet satisfactorily understood. This includes point defects as well as extended defects, such as dislocations and precipitates. Of special interest are investigations of the formation and incorporation mechanisms during crystal growth, including measurement of critical shear stresses for dislocation motion in variously doped

GaAs, and in situ observations during crystal growth. The relation of defect formation to stoichiometry and stoichiometric inhomogeneities, as well as to doping with impurities, deserves special attention.

Among the tools for these investigations will be the powerful electron microscopes of the National Center for Electron Microscopy (NCEM) at Lawrence Berkeley Laboratory; the 1.5-MeV High-Voltage Electron Microscope (HVEM) and the new 1.0-MeV Atomic Resolution Microscope (ARM) are available for such studies. Also of great value will be the technique of x-ray topography, with the aim of in situ imaging of melting and regrowth processes, using either the proposed Advanced Light Source at LBL or other synchrotron radiation sources. Special attention should be given to analytical techniques for detecting impurities, measuring impurity distributions, and determining the stoichiometry; techniques such as neutron activation, charged-particle activation, and heavy-ion Rutherford backscattering will be used.

Electronic Properties of Defects

Identifying both shallow and deep-level defects and establishing their relation to device properties are the major goals in understanding the electronic properties of defects. Specific problems are understanding and controlling the compensation mechanisms in semi-insulating GaAs and the thermal stability of lattice defects involved in these compensation mechanisms.

Among the conventional characterization techniques to be used are the Hall effect, deep-level transient spectroscopy (DLTS) and optically excited DLTS, photoluminescence, optical absorption, including Fourier transform infrared spectroscopy, and electron paramagnetic resonance. In addition, novel techniques such as photothermal ionization spectroscopy, photothermal reflection

spectroscopy, photoacoustic microscopy, and photoluminescence excitation spectroscopy using a tunable dye laser will be used. Special attention will be devoted to making laterally resolved measurements combined with structural information obtained from the same wafers.

GaAs Interfaces—Structural Information

Of major concern in the development of GaAs-based VLSI circuits are the structure and electronic properties of interfaces between the GaAs crystal and other media. The electronic interface states of primarily intrinsic origin present in high concentration deserve special research efforts. Existing analytical techniques that are applicable to the study of surfaces and interface layers include secondary-ionization mass spectroscopy, scanning Auger spectroscopy, x-ray photoelectron spectroscopy, Rutherford backscattering spectrometry, and scanning electron microscopy. These are currently accessible to the NCAM Electronic Materials Program.

In addition, a vacuum tunneling microscope operating at temperatures between ~10 and 400 K will be constructed for the study of surface defects, crystal growth, and the distribution of adsorbed atoms. The study of in situ oxidation of GaAs – a process that is of great technical importance but poorly understood and difficult to control – will be attempted with the tunneling microscope and Raman scattering. Layered structures and near-surface properties will be studied with a variety of particle beam techniques, including channeling, nuclear reactions, and heavy-ion Rutherford backscattering.

APPLICATIONS AND NOVEL DEVICE CONCEPTS

40-574 O - 85 - 86

Gallium arsenide and other Group III-V compounds and alloys offer a wide range of potential applications, including high-speed electronic, optoelectronic, and photovoltaic devices. The full extent of such potentials has not yet been realized, because of materials-related problems. These problems will vary continuously through the development phase of many future devices. Close contact with individuals in leading device-development programs will be sought in order to adjust the research program as needed.

INDUSTRY INVOLVEMENT

The planners of NCAM hope to pioneer a new era of cooperation in the national interest among industry as a whole, individual companies, and the national laboratories. NCAM will accomplish this goal by performing fundamental, long-term research that will expand the knowledge base relevant to materials synthesis, processing, characterization, and use. The results should give U.S. industry as a whole a boost, without explicitly favoring individual companies.

The focus of the Electronic Materials Program has been defined after extensive discussions with GaAs experts at Bell Laboratories, Hewlett-Packard Laboratories, IBM, T.J. Watson Research Laboratories, MIT, the Naval Research Laboratory, XEROX PARC, and others. Unanimous agreement has been found that the development of large-diameter, low-defect-density, high-purity, semi-insulating GaAs crystals is of the greatest importance. We acknowledge the help of several staff members of Hewlett-Packard Laboratories and their interest in a fruitful collaboration. We are looking forward to broadening such interactions with industry.

MILESTONES

Much of the first year of this program will be devoted to detailed planning, equipment design, construction, and requisition. By the ends of the following three fiscal years, we expect to reach the following goals:

FY84:

- Design or substantial modification of a commercial advanced Czochralski-type crystal puller
- Development of a numerical modeling program for crystal growth
- Design of the thin-film interface morphology experiment
- Upgrade of molecular beam epitaxy facilities
- First results on cross-sectional transmission electron microscopy (TEM) studies of ion implantation defects
- Completion of deep-level transient spectrometer (DLTS), electron paramagnetic resonance (EPR) spectrometer, and photoluminescence (PL) apparatus
- Evaluation of x-ray topography using synchrotron radiation
- Assembly of vacuum chamber for surface-tunneling microscope; design of microscope 50% completed

FY85:

- Completion of crystal puller; possibly first crystal-growth experiments underway

- Completion of numerical modeling program for crystal growth; first results for some simple growth conditions
- Results of the thin- film interface morphology experiment
- Atomic resolution and TEM studies of dislocations in GaAs
- First characterization of defects in GaAs by DLTS, EPR, PL, and photoluminescence excitation (PLE) spectroscopy
- Completed design of surface-tunneling microscope

FY86:
- Routine GaAs bulk crystal growth
- Feedback of numerical modeling on crystal growth
- Most characterization techniques established
- Development of laterally resolved electrical and optical characterization techniques
- Completed construction of surface-tunneling microscope

ELECTRONIC MATERIALS
BULK CRYSTALS
GaAs
Thermodynamics of Crystal Growth
New Compound Semiconductors
THIN LAYER AND SURFACES
Interfaces and Thin Film Reactions
Molecular Beam Epitaxy
Deposition Techniques
CHARACTERIZATION
Electrical
Optical
Particle Beams
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Pub-5107

WORKSHOP ON CAM PROGRAM ON POLYMERS AND POLYMER COMPOSITES

Lawrence Berkeley Laboratory

October 24–25, 1983

Chairman

Morton M. Denn

October 1983

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

This work was supported by the U.S. Department of Energy
under Contract No. DE-AC03-76SF00098

Contents

EXECUTIVE SUMMARY 1
Project areas 2
Liquid crystal polymers 2
Composites 2
Polymer-solvent-nonsolvent interactions 2
Block copolymers 2

WORKSHOP PROGRAM 3

PRESENTATIONS 6

LIST OF ATTENDEES 8
UCB/LBL List of Attendees 12

Working Group on Polymer Liquid Crystals 14
Chairman: Manuel Panar

Working Group on Block Copolymers 16
Chairman: Joram Diamant

Working Group on Polymer Composites 17
Chairman: George N. Hartt

Working Group on Polymer/Solvent/Nonsolvent Interaction 18
Chairman: J.D. Moseley

Working Group on Industrial Interaction 19
Chairman: James Economy

Working Group on Program Growth 21
Chairman: Robert J. Samuels
Processing 21
Physics and Physical Properties 21
Chemistry and Chemical Synthesis 22

Appendix A: Planning Document for the CAM Program in Polymers and Polymer Composites 23

40-574 O - 85 - 87

EXECUTIVE SUMMARY

The Polymers and Polymer Composites Program (PPCP) of the Center for Advanced Materials (CAM), Lawrence Berkeley Laboratory, held a workshop at LBL on October 24 and 25, 1983, for the purpose of reviewing CAM-PPCP research plans. In view of the charge to CAM to carry out fundamental research in advanced materials that is relevant to the needs of American industry, invitations to participate were sent to a representative group of industrial scientists and engineers with experience and program responsibility within the general scope of the CAM-PPCP. The workshop was attended by twenty-four participants not affiliated with LBL or the University of California, Berkeley (UBC), twenty-one from the private sector.

The overall focus of the CAM-PPCP as conceived during the initial planning stages is on the generic problem of predicting microstructure during the processing of advanced polymeric materials. The specific research projects selected within this context for the start-up years were based on the capabilities and experience of current UCB and LBL staff. Research was planned on structure development during processing of three materials types: thermotropic liquid crystal polymers, short-fiber composites, and block copolymers. Three processing areas of broad interest in structure development were also selected for study: molecular-weight distribution control, coprocessing, and polymer-solvent-nonsolvent interactions; the last of these has a specific application in polymer membranes, though the broader context is of interest.

The two-day workshop was planned to serve two purposes. First, through talks by recognized experts in the program areas, the state-of-the-art was to be defined and significant unresolved research problems identified. Then, the CAM-PPCP research plans were to be presented and evaluated within the context of the state-of-the-art presentations in several working groups. The overall conclusion of the workshop was a strong endorsement of the program philosophy and of the program plans during the startup period. This was coupled with a strong consensus for the need to add personnel in two essential areas not covered by individuals currently at LBL or UCB.

There was general agreement that the research areas selected for the start-up period are appropriate, in that they represent research in advanced materials of significance to American industry where important generic problems remain to be solved. Specific recommendations regarding program areas follow a brief discussion of concerns regarding staffing and policy.

There is no one with expertise in polymer structure characterization at LBL or UCB, with the important exception of nuclear magnetic resonance, and in the properties of solid polymers.

The former was identified as an essential short-term need, and the latter as a longer-term need.

Similarly, there is no expertise at LBL or UCB in the synthesis of well-characterized polymers, and the program is dependent on industrial sources of materials. There was a strong consensus that in-house synthesis capabilities are required.

There was considerable concern over the apparent lack of present definition of patent policy with regard to industrial participation, and there was a belief that industrial participation would be slowed until the policy question was resolved. Possible modes of industrial participation will depend on the details of the final patent policy.

Project areas

Liquid crystal polymers.

Support for the program plans was very strong, both with regard to significance of the particular research and the feeling that CAM was the appropriate place to carry it out. The area was cited in the Working Group summary as among the most exciting and important of recent developments in polymers.

Composites.

Discussion here was far-ranging, given the broad scope of the subject. There was general agreement that the problems to be studied were important and appropriate, but limited in scope. The need to integrate the focus on process-induced structure with work on solid-state polymer structure/properties was emphasized.

Polymer-solvent-nonsolvent interactions.

The focus on the generic problem of phase separation was supported as appropriate and important, with the observation that this is closely coupled to similar problems in the block copolymer area. The group felt that the membrane work in the future should include research on the problem of membrane separation mechanisms.

Block copolymers.

It was felt that work on block copolymers is important because of their expected large role in the technologically important area of polymer blends or alloys. The present plans were viewed as appropriate, but too narrow in scope, with a recommendation that more of a focus be placed on experimental studies of the interphase and on multiblock copolymers, as well as on solid state properties of block copolymers.

WORKSHOP PROGRAM

Monday, October 24

9:00 - 9:30	Overview of Lawrence Berkeley Laboratory David A. Shirley, Director of LBL
9:30 - 10:00	Overview of the Center for Advanced Materials Kenneth S. Pitzer, Acting Director of CAM
10:15 - 10:30	Workshop Objectives Morton M. Denn, Group Leader of CAM-PPCP
10:30 - 11:30	Polymer Science and Engineering: Challenges, Needs, and Opportunities Rudolph Pariser Central Research and Development Department E.I DuPont de Nemours & Co.
1:00 - 2:00	Composite Materials R. Byron Pipes Center for Composite Materials University of Delaware
2:00 - 3:00	Liquid Crystal Polymers Michael Jaffe Celanese Research Co.
3:15 - 4:15	Block Copolymers Dale J. Meier Michigan Molecular Institute
4:15 - 5:15	Polymer Membranes Harold K. Lonsdale Bend Research Inc.
6:00 -	Reception and Dinner

Tuesday, October 25

8:30 - 10:30	CAM-PPCP Plans
8:30 - 8:40	General Overview - Morton M. Denn
8:40 - 9:15	Liquid Crystal Polymers - Morton M. Denn and Jeffrey A. Reimer
9:15 - 9:35	Block Copolymers - Clayton Henderson
9:35 - 9:55	Polymer-Solvent-Nonsolvent Interactions - David S. Soong
9:55 - 10:20	Short-Fiber Composites and Co-Processing - Morton M. Denn
10:20 - 10:30	Polymer Reaction Engineering - David S. Soong
10:45 - 12:00	Working Session I Liquid Crystal Polymers Chairman: Manuel Panar E.I. DuPont de Nemours & Co.
	Block Copolymers Chairman: Joram Diamant Hexcel Corporation
1:30 - 2:30	Working Session II Polymer Composites Chairman: George N. Hartt Owens-Corning Fiberglass Corp.
	Polymer-Solvent-Nonsolvent Interactions Chairman: J.D. Moseley Dow Chemical USA
2:40 - 3:40	Working Session III Industrial Interaction Chairman: James Economy IBM Research Laboratory
	Program Growth Chairman: Robert J. Samuels Georgia Institute of Technology
4:00 - 5:30	Working Group Reports by Group Chairmen
5:30 - 7:00	Reception and Wine Tasting.

Format

Working groups were organized in parallel sessions. Each participant was asked to serve on one particular working group, and then to choose any two others in which to participate. Graduate students associated with the CAM-PPCP acted as working group secretaries and prepared draft group reports, based on their own notes of group discussions and transcripts of the reports by the group chairmen, with final editing by the working group chairmen.

PRESENTATIONS

Speakers presenting state-of-the-art talks were not asked to prepare manuscripts, since the main purpose of the talks was to establish a context for discussion of the proposed CAM program. Three of the speakers were invited specifically to present reviews similar to those prepared for other audiences, and manuscripts of these reviews are available. Rudolf Pariser's talk was based on the study by the National Research Council Panel that he co-chaired. References for these manuscripts are as follows:

POLYMER SCIENCE AND ENGINEERING: CHALLENGES, NEEDS, AND OPPORTUNITIES
Ad Hoc Panel on Polymer Science and Engineering
Committee on Chemical Sciences
Assembly on Mathematical and Physical Sciences
National Research Council
National Academy Press
Washington, D.C. 1981

Available from

Office of Chemistry and Chemical Technology
National Research Council
2101 Constitution Avenue, N.W.
Washington, D.C. 20418

ANISOTROPIC POLYMERS. THEIR SYNTHESIS AND PROPERTIES
Gordon W. Calundann and Michael Jaffe
The Robert A. Welch Foundation Conferences on Chemical Research
Research Conference XXVI. Synthetic Polymers
Houston, Texas, November, 1982.

THE GROWTH OF MEMBRANE TECHNOLOGY
H.K. Lonsdale
Journal of Membrane Science
10 (1982) 81-181

The presentations by CAM-PPCP speakers were based on material contained in a Planning Document provided in advance to all participants. The text of the Planning Document is attached as Appendix A.

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Prepared 11-07-83

Working Group on Polymer Liquid Crystals
Chairman: Manuel Panar

Liquid crystalline structures leading to highly ordered, high strength organic polymeric materials is one of the most exciting advances in the last 15 to 20 years in polymer science. In this area, as in much of polymer science in America, the research initiative has been in industrial laboratories, and technology has been leading science. It was the view of the Working Group that it was very important that non-industrial research laboratories such as this one apply a broader, perhaps longer range, viewpoint in order to establish the basic science underlying the developing technology. The development of this basic science will provide the ideas that will define the directions of industrial development in the future. The research proposed in the planning document is consistent with this point of view, and the proposal is particularly timely and important. In spite of the vast amount of work going on, we are not aware that the type of program that has been proposed is being carried out anywhere.

The discussion of specific technical issues regarding anisotropic melts focused on identifying the scientific bottlenecks to the advancement of the field. The first issue is the structure of the melt, which is a very difficult problem. New probes are needed, and it was suggested that this might be an area where the advanced light source may have some unique applications in the polymer world. The question of structure includes definition of the distinction between the various hypotheses regarding the presence of domains versus correlation volumes without definite boundaries. The second issue is the question of the determination of the order parameter in the nematic phase.

The structural changes that take place under shear or elongation are critical to the morphology distribution of the solid polymer and are central to the program that has been proposed by CAM. There are two parts to this problem. First, there is the understanding of the normal changes that might be expected from an oriented system under shear or elongational fields. Second, there is the question of phase change. What is the effect of the shear field on the transition from an isotropic to nematic structure?

An additional item that was discussed was the unknown effect of molecular weight distribution of anisotropic melts on the rheology, the nature of the phase diagram, and on the structure of the liquid.

Finally, there was discussion of the structure of liquid crystal polymer fibers, and the relationship of the structure to mechanical properties. This last area is not covered within the current definition of the CAM program.

WORKING GROUP ON BLOCK COPOLYMERS
CHAIRMAN: JORAM DIAMANT

Working Group participants agreed that the fundamental approach proposed by CAM is most likely to maximize the benefits of the program. There was general agreement that there is considerable potential for long term growth in the development of a predictive capability for block copolymer rheology, and the proposed programs in this area were felt to be technically sound and to represent attainable goals of practical utility as well as fundamental scientific value.

Participants felt that the planned program on block copolymer melt rheology should be extended to include models for the mechanical properties of solid block copolymers. There was felt to be an overemphasis on the theoretical problems associated with the interphase region, which is emphasized in both the thermodynamics and rheology, and it was felt to be important to develop experimental means of verifying interphase structure. Solid state NMR was thought to be one possible experimental tool for elucidating interphase structure, and the advanced light source should be useful for obtaining short-time data during deformation of the interphase regions.

It was felt that multiblock copolymers represent an important area of research, and that it would be appropriate to move into this area at this time, even before the AB and ABA block copolymers are fully understood. Prediction of some applied properties, such as those under large deformations, is another important area worth exploring.

Block copolymers are expected to play a major role in the technologically important area of polymer blends, and it was felt that CAM should develop a program to examine the interfacial activity of block copolymers in blended systems.

It was also recommended that the effect of molecular weight distribution and block size distribution on bulk properties be studied. In addition, the program can be extended to investigate block copolymer films with oriented domains; these materials may find useful applications.

Finally, all Working Group participants felt that an in-house ability to synthesize model compounds in meaningful quantities is essential for the long-term health of the program.

Working Group on Polymer Composites
Chairman: George N. Hartt

The Working Group concluded, with some qualifications, that the proposed research program in short fiber composites represents a good starting point for a program in composites, with the program to be modified in the future with advice from industrial users and in response to developments in composite technology. The goal of the CAM program should always be to identify generic problems, address them, and leave it to industry to specialize the results for particular needs.

There was considerable discussion over the question of whether short fiber composites represent an advanced material. Participants had a range of definitions of "advanced material," but it was generally agreed that under one definition or another short fiber composites are advanced materials and their study is appropriate. Several research areas beyond those outlined in the proposal and considered to be of significant industrial importance were discussed: mechanisms of fiber breakage during processing; the role of the composite matrix in load bearing, durability, and aging; and the influence of the interphase/interface between matrix and filler. (It was suggested that perhaps the surface science program might be the appropriate place to study questions regarding interactions between matrix and filler, but the Working Group generally supported incorporating such research in the Polymer/Polymer Composites Program.)

The most serious deficiency seen in the proposed program, and relating to some of the topics listed above, is the lack of any expertise in solid mechanics. There was some discussion as to whether the area of solid mechanics might best be handled through collaboration with other composites research programs focusing more on the solid state, but there was general agreement that at least one senior investigator resident at CAM is required in order to meet the need of predicting and obtaining solid structure-property relationship.

Finally, there was some discussion regarding the study of more general heterophase systems, including ceramics and metals, with the thought of integrating several CAM programs into a focus on one generic problem.

Working Group on Polymer/Solvent/Nonsolvent Interactions
Chairman: J.D. Moseley

During the last decade there has been a growing interest in the field of membrane technology. From the period starting about 1979, a large component of the increase in the patent literature has been in Japanese patents, both in Japan and in the United States. Moreover, it was announced about a year ago that membranes would be highlighted among the areas of particular interest to the MITI organization mission. There are a variety of types and uses of membranes; the fundamental question of polymer/solvent/nonsolvent interaction is broadly relevant to the problem of structure formation in porous membranes.

It was the consensus of the group that the research program proposed by CAM represents a good beginning and should continue essentially as outlined, with continuing discussion with interested industry representatives in order to help focus some of the questions that are being asked. Research on this generic problem might be coordinated with other related CAM projects.

The group recommended that a high priority future thrust is to study the question of why polymer films separate, with a goal toward establishing the relationship between the separation mechanisms and the detailed morphology.

The group felt that there might be a unique opportunity to utilize LBL strength in radiation capability to study the use of high energy radiation to modify membrane surfaces. The outer thousand angstroms of the membrane provide the discriminating layer in most cases, so modification of surface features like density and crosslinking might offer new possibilities with regard to both performance and understanding of mechanisms.

Finally, it was felt to be important to establish performance and quality tests in this area, in order to establish how one knows when he has accomplished what he has set out after.

Working Group on Industrial Interaction
Chairman: James Economy

The group discussion began by examining the modes of interaction between CAM, industry and the Department of Energy. The primary intent of this activity will be to generate basic knowledge in polymers and to transfer that knowledge to industry. It was noted that this does represent the first time that DOE has supported a major polymer activity, and hence there is probably not a great deal of experience in the DOE organization to enable evaluation of a polymer program. The CAM polymer group will therefore have to make a particular effort to establish the appropriate interactions with DOE as well as with industry. It was also noted that the DOE Basic Energy Science materials programs have not had a very good track record during the past decade in technology transfer, as opposed to the weapons laboratories.

Exchange of personnel between CAM and industry was seen to be an important mode of interaction. The group felt that it was very important that the flow be in two directions: not only should industrial people come to CAM for periods of a few months to a year, but CAM personnel should also spend time in industry, perhaps on sabbatical leave. Exchange of personnel is probably the most effective means of establishing collaborative research, including joint supervision of research students or postdoctoral fellows. Other modes of industrial interaction that were recommended include the establishment of an advisory board of industrial scientists and continued sponsorship of workshops and symposia.

Industrial sponsorship was discussed as possible mode of interaction. It was generally felt that industrial involvement in projects such as CAM is greater when a financial commitment has been made. There was a concern, however, that an emphasis on industrial financial support could serve to hinder collaboration with companies that were not prepared or able to make a financial commitment to the program. It was noted in this connection that the sponsoring companies of the Center for Composite Materials at the University of Delaware all have sales of at least $100 million per year.

There was considerable concern expressed about the impact of the DOE patent policy on industrial collaboration, even to the extent of the ability of industrial scientists to involve themselves in CAM activities when no corporate financial support was involved. There was concern over the apparent lack of present definition of a patent policy, and a belief that industrial participation would be slowed until the policy question has been resolved. Possible modes of industrial participation will ultimately depend on the details of the final patent policy for CAM.

Other modes of interaction that were recognized as important, but received less discussion, included publication, mutual access to experimental facilities, and industrial preparation of materials for testing. Finally, it was felt that research by the polymers group in broader problems involving the ceramics and metallurgy communities would be highly desirable.

Working Group on Program Growth
Chairman: Robert J. Samuels

It was the general consensus of the working group that the program goals require expansion in two areas:

1. Characterization of the structure and properties of polymers and polymer composites in the solid state.
2. Synthesis of well-characterized polymers.

The specific recommendations that follow are directed to the three main program subdivisions as described in the CAM planning document: Processing, Physics and Physical Properties, and Chemistry and Chemical Synthesis.

Processing

It was generally accepted that the overall thrust of the processing portion of the program was quite satisfactory. It was noted that the current expertise in the area of numerical computation is provided by a UC Berkeley Miller Fellow on a two-year appointment. The central role of this area of expertise for the analysis of processing and design calls for the appointment of a senior staff member specializing in numerical computation within about a two-year time frame.

It was suggested that the research on the various anisotropic and orientable materials being studied might be enhanced by the utilization of electrical or magnetic fields in conjunction with flow experiments.

Physics and Physical Properties

This is an area in which considerable effort is required. The thrust of the polymers and polymer composites program is to develop the understanding necessary to produce polymeric objects having desired properties, which require the ability not only to predict structure but also to establish a frame of reference in which to determine desirable structures. In that regard it was felt that there is an immediate need for the addition of a senior level person with research expertise in structure determination, followed subsequently by a second senior appointment in order to ensure adequate coverage of both the structure determination and structure-property

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areas. The sophisticated equipment necessary for structure and structure-property research will also require a full-time technical instrument technician. The Working Group felt that it was important to have access to certain in-house equipment. In-house wide angle x-ray for orientation studies would be very useful because of the slow nature of these measurements. Small angle x-ray was considered to be almost essential. It was the understanding of the group that there are already plans for in-house NMR, and this acquisition is supported. Fluorescence equipment was considered to be very desirable as long as the molecular systems to be studied have backbone fluorescent molecules. Other recommended pieces of in-house equipment include FTIR, an osmometer for absolute molecular weight determination, and GPC with auxiliary detectors.

Chemistry and Chemical Synthesis

All Working Group members felt that the ultimate viability of the CAM polymer program would require an in-house ability to synthesize model compounds for further study, and it was highly recommended that one senior synthetic chemist join CAM as soon as facilities permit. Some industrial persons on sabbatical may want to visit CAM for a year to assist with model compound synthesis. Graduate student training in this area may be supported by associate industries.

APPENDIX A
PLANNING DOCUMENT FOR THE CAM PROGRAM IN POLYMERS AND POLYMER COMPOSITES

INDEX

BACKGROUND 26
MOTIVATION 28
Liquid Crystal Polymers 28
Fiber-Filled Polymer Composites 29
Block Copolymers 30
Polymer- Solvent- Nonsolvent Interactions 31
Co-processing 33
Molecular Weight Distribution Control 33
SCIENTIC PROGRAM 34
Liquid Crystal Polymers 36
Fiber-Filled Polymer Composites 38
Block Copolymers 41
Polymer- Solvent- Nonsolvent Interactions 43
Co-processing 45
Molecular Weight Distribution Control 46
PARTIAL FACILITIES LIST 47
CURRICULUM VITA 48

PLANNING DOCUMENT

Program in Polymers and Polymer Composites

National Center for Advanced Materials

Lawrence Berkeley Laboratory

SUMMARY

The planned polymer and polymer composites program at NCAM will focus on the generic problem of predicting microstructure during processing. Research during the start-up period will deal with the following problems: processing of liquid crystal polymers, fiber orientation and matrix stress in short-fiber composites, rheology and thermodynamics of block copolymers, structure control through polymer-solvent-nonsolvent interactions, co-processing, and molecular weight distribution control.

Background

The manufacture of articles from synthetic polymers now has a long history, but it is only recently that high-performance polymeric materials have become a reality. Materials are now being synthesized, for example, with strength, thermal stability, and chemical resistance sufficient to consider their use as lightweight structural elements in a variety of environments.

The properties of objects made from polymeric materials depend not only on the chemical composition of the polymer and the properties of any filler (e.g., glass fibers), but also on the entire history of each material element during processing. It is the latter that establishes the detailed morphology throughout the shaped object, and it is the morphology that ultimately determines the end-use properties. (For example, ultra-high tenacity polyethylene filaments do not differ chemically from filaments with breaking strengths an order of magnitude lower that have been made from the same polymer batch; they simply have been processed differently.) There are a number of fundamental relationships, unique to each polymer or polymer composite system and to each processing geometry, that determine final properties:

1) The dependence of the rheology (determination of the local stress by the deformation and thermal history) during processing on the material composition.
2) The interaction of rheology with processing conditions and geometry in determining the microstructure of the final product.
3) The way in which macroscopic end-use properties depend on the microstructure distribution.

Chemical structure and material composition will determine such factors as resistance to chemical and thermal degradation and the theoretical limits of

mechanical properties, and hence appropriate end-uses. Chemical structure will also determine the bounds of processing temperatures and the equilibrium state of the solid polymer: amorphous or slightly or highly crystalline, for example. The factors outlined above are the predominant ones, however, in establishing the properties of a particular material composition in a particular shaped object, including the extent to which the equilibrium solid state structure is attained.

There is a pressing need to make progress on the generic problem of predicting microstructure distribution during processing. The specific aspects of this generic problem differ for different types of polymer and polymer composite materials and for different classes of processes, but in broad terms it is necessary to incorporate the complex rheology, equilibrium thermodynamics, and phase transition kinetics with a description of system geometry, fluid mechanics, heat transfer, mass transfer, and even aerodynamics in the analysis of processing steps such as compression or injection molding and fiber and film extrusion. The structure of the final product will vary with position as a result of the interaction of these material and processing variables. An example is the fiber orientation distribution and residual matrix stress in molded short-fiber composites. It is not currently possible in most areas of polymer technology to predict the structure distribution.

In classifying the focus of our research efforts, it is useful to distinguish research on specific classes of materials from specific types of processes, although there is of necessity a degree of overlap. Our initial focus will be on three classes of polymeric materials having considerable applications potential: liquid crystal polymers, block copolymers, and short-fiber polymer composites. We will also initiate research in three processing areas: co-processing, structure control through polymer-solvent-nonsolvent

interaction, and molecular weight distribution control through polymerization reaction engineering.

MOTIVATION

Liquid Crystal Polymers. Liquid crystal polymers (LCP's) are macromolecules that might be characterized as rod-like, with relatively rigid backbones; they possess mechanical properties in the fluid phase that are generally like those of fluids, yet are sufficiently structured to transmit polarized light. Fibers prepared from liquid crystal polymers have high modulus and tenacity, and the materials show superior thermal stability and resistance to chemical attack relative to conventional industrial polymers. The only LCP that is generally commercially available is DuPont's Kevlar$^{(R)}$, which appears to be poly (1,4-phenylene terephthalamide). The reported modulus and tensile strength of Kevlar$^{(R)}$ 49 fibers are roughly equal to those of steel. PPT decomposes before it melts, and it must be processed in a concentrated sulfuric acid solution. This restricts applications to the manufacture of fibers, where the solvent can be removed through a wet or dry spinning process. Molded parts exploiting the superior physical properties are not possible.

Melt processible LCPs are known, and some copolymers of aromatic polyesters appear to have properties that would enable their use for high-performance applications as both fibers and engineering plastics. Fibers drawn from the liquid crystal polyesters tend to be highly oriented, almost certainly because of the liquid crystal structure in the melt, and nearly all of the orientation is believed to occur during extrusion; this is in contrast to the behavior of conventional flexible-backbone polymers, where most of the orientation development occurs during the drawing process.

The rheology of LCPs is highly complex, and there is no generally-accepted theoretical framework currently available for making predictions for use in processing flows. There is a "domain" structure at low deformation rates that causes fluid responses reminiscent of heterogeneous systems. There appears to be a natural length scale for low molecular weight liquid crystals at which the bulk rheological properties become dependent on the size of the apparatus, and limited data on LCPs are suggestive of a size dependence.

The onset of flow instabilities is usually the limiting factor in polymer processing operations. The most important instabilty from a processing point of view is melt fracture, which is a breakdown of steady flow through an extrusion die. It is probable that new flow instabilities that are unknown in flexible polymers will occur with LCPs. Spatial instabilities have been observed for low molecular weight liquid crystals. A "herringbone" pattern has been observed in shear flow of some LCP solutions, where the system breaks up into bands with molecular alignment at ±45° to the flow direction. Studies of the breakdown of simple streamline flow for LCP melts have not been reported, but we have seen injection molded samples that show surface textures suggestive of a more complex flow in the mold than that usually observed with common engineering plastics.

Fiber-Filled Polymer Composites. Chopped fibers, typically of glass, are commonly used to form composites with both thermoplastic and thermosetting polymers. Many parts of an automobile, including structural components, could be made from such composites with considerable savings in weight over the use of steel. The fiber density and orientation are known to vary across even a simple molded part. The bulk mechanical properties of the composite can be predicted if the fiber orientation is known, and shrinkage can be estimated if the stress distribution in the polymer matrix is known. Prediction of the

fiber orientation and stress distributions for most processing flows is not possible at present. The bulk rheology of molding compounds even without fibers is not well-understood.

Current theories of the flow of fiber-filled systems allow prediction of orientation only in the limiting case of a dilute suspension in a simple suspending medium, which is of no practical interest. The expected behavior of fiber-filled systems can be characterized in terms of volume fraction of fibers, ϕ, and particle aspect ratio, R, as follows:

$\phi R^2 \ll 1$ non-interacting

$\phi R \ll 1$ but $\phi R^2 \ll 1$ sporadic interactions

$\phi R \sim 1$ substantial interaction

The substantially-interacting regime will occur for $\phi \ll 1$ for most fiber-filled systems, and hence is nearly always the situation of interest. Macroscopic structures will be developed in some flow fields when there are strong interactions, and there is no theoretical framework for determining the buildup and breakdown of such structures, or their effect on bulk rheology. Continuum theories of orientable systems do exist, and are quite similar to those used to describe low-molecular weight liquid crystals, but no solutions to meaningful flows have been obtained to date because of the numerical complexity. It is unlikely in any event that these theories for "transversely isotropic fluids" will be adequate to describe the development of orientation during the deformation of highly-filled composites, since multiple-particle interactions appear to be unaccounted for.

Block Copolymers. Copolymers formed from two or more monomers can be prepared in random or block form. The behavior of random copolymers is essentially like that of the homopolymers, but block copolymers form microphases on a scale of about 300 angstroms and show radically different

behavior. The solid state mechanical properties of block copolymers resemble those of crosslinked systems, but the absence of chemical cross-linking allows liquefaction and reprocessing with heating without material degradation. The presence of the microphases endows the sample with the characteristics of a composite, but failure cannot occur at a "phase" boundary since the bonding is covalent. Similarly, while two-phase blends of homopolymers will tend to fail at the interface, a block copolymer will dissolve in both phases, "gluing" the system together thermodynamically. When added to one of the homopolymers the block copolymers will migrate to the exterior surface, thus creating a surface with properties different from the bulk.

The mechanical properties of block copolymers are determined by the detailed solid state structure. Experiments show the existence of an "interphase", the properties of which can be altered by the use of solvents favoring either of the homopolymer blocks. The microstructure is sensitive to processing temperature, block composition, and polymer/solvent compatability, as well as to the stresses encountered during processing. Existing microphase thermodynamics theories cannot explain the non-symmetric interphase composition profiles and interblock "mingling" in the pure phases observed experimentally, nor is the microphase separation theory satisfactory except in the limit of solvents equally good for both blocks. No theory currently exists to predict the complex fluid rheology, even if the microstructure at rest is well characterized.

Polymer-Solvent-Nonsolvent Interactions. Polymer membranes with complex, controlled morphologies are generally produced by a multi-step process based on intimate interplay of the macromolecules with solvents and nonsolvents. A concentrated polymer solution dissolved in a good solvent is first cast on a flat surface. It then undergoes a step-wise coagulation via contact with a

nonsolvent, followed by drying. The final structure can range from a totally porous membrane to an asymmetric (anisotropic) one with or without finger formation. Asymmetric structures with a continuous gradient of pore sizes spanning the membrane are currently the most widely used designs in commercial applications of membrane technology, with dialysis, electrodialysis, reverse osmosis, ultrafiltration, gas separation, and biological reactions with entrapped microorganisms representing some few examples. The exact conditions under which the multi-step process is carried out determine the resulting membrane morphology and properties. The process entails a complicated change of state and can be described at least in part by trajectories in a phase diagram. Mass-transfer limitations governing the relative rates of diffusion of the small molecules also play a critical role in membrane formation, as thermodynamic equilibrium is not necessarily achieved everywhere during preparation.

Similar polymer-small molecule interactions play a central role in the development of resists in microelectronics fabrication. Of particular interest are the positive resists, which suffer molecular degradation and chain scission during exposure to radiation. Upon contact with a mixed developer of solvent-nonsolvent pair, the irradiated region is selectively removed, leaving the unexposed region of the film covering pre-determined parts of the substrate in subsequent processing steps. The rate of development, contrast, and topography of the resulting pattern depend strongly on the intricate polymer-solvent-nonsolvent interactions and associated mass-transfer limitations. Hence, a firm understanding of how the solvent-nonsolvent pair influences polymer coil conformation, which in turn affects the rates of penetrant diffusion and phase separation, is vital.

Co-processing. Co-extrusion and co-molding of two polymer melts, or a polymer and a polymer composite, is an area of growing interest and importance. In a typical application, one might wish to mold a piece with a composite core, for structural purposes, and a polymer "skin" for appearance, chemical resistance, or other purpose. The usual problems associated with prediction of structure resulting from the flow of a rheologically-complex material in a mold exist here, but they are compounded by the basic problem of control of the location of the interface. Interfacial motion might occur because of classical hydrodynamical instabilities, but it is more likely that the movement observed in processing is simply a consequence of the stress distribution induced by the hydrodynamics and the rheology of the two phases. A prototypical problem that is not currently understood is the tendency of a more viscous core material to migrate to an obtuse sharp corner in a mold, causing a depletion of the skin material in that region. Such migration might be a normal flow pattern for co-current flow of viscous fluids, or it might be a manifestation of the viscoelasticity of the polymeric liquids; the latter seems more probable, since the observation is contrary to the encapsulation by the lower-viscosity fluid that is normally expected.

Molecular-Weight Distribution Control

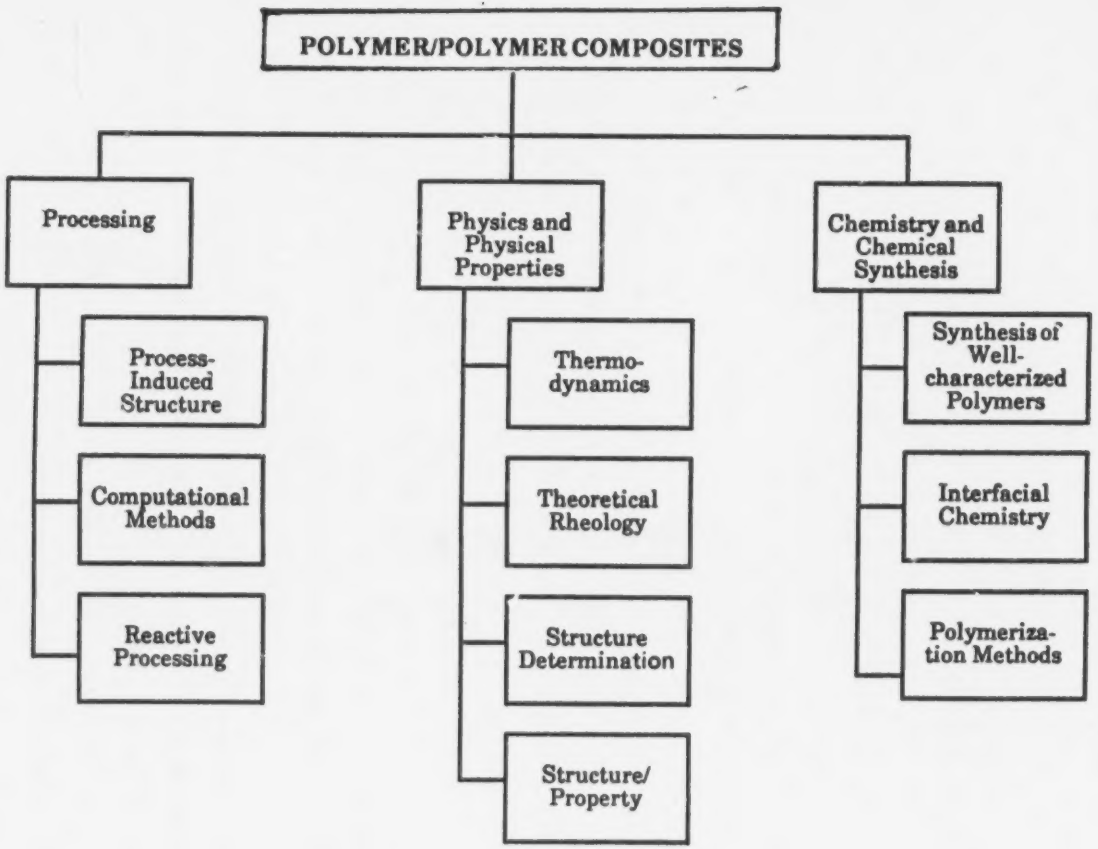
The most difficult problems in the design of liquid-phase polymerization reactors to produce polymer of a desired molecular weight, molecular-weight distribution, branching, and co-polymer composition distribution along the chain are associated with the exothermic nature of polymerization reactions and the large viscosity buildup with conversion. Temperature control is difficult because of the low thermal conductivity and difficulty of mixing. Methods other than bulk polymerization have been employed to overcome these problems, including suspension, emulsion, and solution techniques. The first two have high impurity levels, whereas the last requires solvent recycle.

Molecular structural characteristics are determined by the history of reaction conditions throughout the polymerization. It is therefore necessary to incorporate the kinetics, heat and mass transfer, and reactor fluid mechanics into an overall description that enables prediction of the development of the macroscopic measures of interest. Within this context, the problem of structure control can be visualized as a problem in optimization, where modern control-theoretic methods of programming reactor conditions can be employed. This approach has seen only limited use to date.

SCIENTIFIC PROGRAM

The description of the scientific program must of necessity focus on plans for the start-up period (say, the first three years), with full recognition that this is a preliminary document prepared prior to the detailed discussions with industrial colleagues. Specific research tasks are planned in each of the program sub-areas related to processing described above. These are discussed in the following paragraphs. The program structure towards which we plan to evolve is shown in the accompanying figure. The specific program tasks that are being undertaken during the start-up period generally encompass more than one organizational subdivision.

The start-up program has been chosen to utilize the backgrounds and facilities of the investigators who are already members of the staff of the Lawrence Berkeley Laboratory and/or University of California, Berkeley. Their scientific backgrounds are described briefly below, together with a list of major equipment currently installed in the UC Berkeley polymer laboratories. The major staff deficiencies are in the areas of structure determination, structure/property relations, and polymer synthesis, and these are the priority areas for future staff expansion. We anticipate a senior staff of


POLYMER/POLYMER COMPOSITES
Processing
Process-Induced Structure
Computational Methods
Reactive Processing
Physics and Physical Properties
Thermo-dynamics
Theoretical Rheology
Structure Determination
Structure/ Property
Chemistry and Chemical Synthesis
Synthesis of Well-characterized Polymers
Interfacial Chemistry
Polymeriza-tion Methods

approximatley eight LBL scientists and UC Berkeley faculty, plus visiting scientists from industry, universities, and other laboratories, graduate research assistants, and post-doctoral fellows.

Liquid Crystal Polymers (Denn/Reimer/Amundsen - GSRA/Moore - GSRA supported by PRF). The thrust of this research is to establish the way in which processing affects the structure of thermotropic liquid crystal polymers. The research will be in two broad areas: structure determination and the relation between structure and the onset of flow instabilities. The latter work will be coordinated with the NCAM program but is separately supported by the Petroleum Research Fund.

A variety of solid state nuclear magnetic resonance (NMR) techniques, including magic angle sample spinning, cross-polarization and high power decoupling, proton multiple pulse and multiple quantum techniques are being utilized to study microstructure in polymers. We plan to utilize NMR to study domain structure and structure change with deformation.

The ability to control proton spin diffusion with multiple pulse techniques has application to the determination of domain structure with extent of processing. Because protons near the boundaries of domains experience more disorder and motion than those at the interior, the former should exhibit much shorter relaxation times. A study of how fast proton magnetization spin communicates along domain edges may reveal information on both size and orientation.

Order parameters within domains may be obtained from a variety of the angular-dependent interactions occurring in the NMR of solids. For example, carbon-13 chemical shifts could be monitored as a function of angle between the external magnetic field and the orientation axis of the polymer by using high power proton decoupling. Both carbon-proton and proton-proton dipolar

interactions provide order parameter information complementary to the chemical shift data. The observation of heteronuclear (or homonuclear) dipolar oscillations allows for the orientation of the molecular coordinate system in the chemical shift principle-axis system which, when combined with the known orientation of the sample within the applied field, leads directly to order parameters. Indeed, this technique has been used extensively to characterize order parameters in partially-oriented biological systems.

If relaxation times at domain edges are significantly different from those within domains, dipolar echo and proton multiple pulse techniques may be used to observe resonances from interfacial regions selectively, and thus allow for motional and geometric characterization of these regions. These techniques may play an important role in the characterization of domain boundaries as a function of particular processing conditions.

In addition to the primary thrust of NMR characterization of structure development during processing, we plan to utilize other methods. Modulus and tenacity of formed samples will be measured using standard techniques, since they provide insight into overall orientation, and x-ray diffraction measurements will be used. We will attempt to use fluorescence polarization to study orientation development in amorphous regions; liquid crystal polymers contain functional groups that are expected to fluoresce, and a preliminary test on borrowed equipment elsewhere was promising.

Rheological characterization of the melt as close as possible to processing conditions is, of couse, essential. This will be done using two new pieces of characterization equipment in the polymer laboratories at U.C. Berkeley: the Model 705 Rheometrics Mechanical Spectrometer, and a computer-controlled servo-hydraulic test machine equipped with an Instron capillary rheometer. The latter system is designed to operate at higher temperatures

and internal pressures than is customary in order to reach the relevant processing range.

The complementary research on conditions for the breakdown of simple streamline flow is supported separately through a grant from the Petroleum Research Fund, effective Sept. 1, 1983. This will involve extrusion experiments through a range of capillaries in order to characterize the onset and nature of fracture. We also plan flow visualization experiments by marking billets and looking at streamlines in the rheometer barrel, prior to the contraction; it is here that we anticipate possible new instabilities for the liquid crystal systems. The high pressures resulting from the very small capillaries necessary to investigate size effects are a confounding factor in such a study; free volume effects will become important, making it difficult to distinguish between characteristic size and free-volume phenomena, but we believe that the relative roles of the two contributions can be separated.

Fiber-Filled Polymer Composites (Denn/Lipscomb - GSRA). This part of the program has as its goal the prediction of orientation distribution and residual matrix stress for the flow of fiber-filled systems in complex processing geometries. The theoretical portion during the early years of the program will focus on the build-up and breakdown of structure in strongly-interacting particulate systems in deformation fields, while the experimental portion will emphasize the rheology and the influence of complex flows on the orientation distribution function.

There is strong evidence of hydrodynamically-induced structures in shearing motions of concentrated particulate suspensions. We believe that the existence of such structures must depend on the presence of deformation gradients induced by boundaries, and will occur at a critical concentration that depends on the particle geometry and the nature of the flow field (e.g.,

we do not expect such structures ever to form in a flow that is essentially extensional). We plan first to study the possible equilibrium configurations of low-order n-tuplets of cylinders confined between walls in a shear field, using both classical lubrication theory and finite-element methods. These equilibria are likely to be unstable, and we will use lubrication theory to study the time scales and modes of structure breakup. (The breakup mechanism is likely to be associated with structure rotation and a "rolling-off" of portions of the structure. A similar mechanism, in qualitative terms, may be responsible for the breakup of domains of polymer liquid crystals in a shear field; indeed, we expect much of the research on fiber-filled sytems and liquid crystals to be mutually applicable in qualitative terms.)

We plan to continue a research collaboration with Prof. David Boger of Melbourne University, using existing facilities at Melbourne, to study fiber orientation distribution and structure formation in complex flows. This will be done by using glass fibers suspended in an epoxy liquid of the same index of refraction, so that flow visualization techniques developed at Melbourne for optically-transparent systems can be employed. The effect of fiber-loading on matrix kinematics will be studied in a channel with a sudden change in cross-section using a new laser-speckle method that requires only a low-powered laser. Fiber motion and interaction will be followed by including a small number of visible fibers, either by coating them or by use of fibers having a different index of refraction.

We will be carrying out complementary experiments of two types at Berkeley. We will use the computer-controlled test machine to study orientation distribution and force-deformation rate relations on squeeze flow of fiber-filled systems. The orientation distribution will be determined optically in solidified molded parts using a Fraunhoffer diffraction

apparatus. It is likely that as we gain insight into the factors that influence orientation, and develop predictive procedures for flow in complex systems (discussed below), we will wish to utilize pilot-scale computer-controlled molding machines for experiments that are industrially relevant.

Predictive ability in mold flow requires an understanding of material rheology that is currently lacking. We plan an experimental study using the Rheometrics Mechanical Spectrometer (and possibly the capillary rheometer) of the macroscopic rheology of systems characteristic of the composition of sheet molding compounds: polyester resin, small particulates (e.g., calcium carbonate), and glass fibers. We wish first to determine the rheological behavior of the unfilled system, followed by filled systems of various compositions. The presence of both small and fibrous particulate filler is expected to lead to rheologically-complex behavior.

We plan also to study the numerical problem of flow of structured materials in complex geometries. This problem area is relevant to both filled systems and polymer liquid crystals. As we have noted, the current level of theoretical understanding of the rheology of structured liquids is limited, and existing theories are applicable only to dilute composite systems. Even here, there are closure problems reminiscent of those in classical statistical mechanics that enter in attempts to write a proper continuum description for the stress and the orientation distribution function. We expect certain aspects of the mathematical structure to remain even for highly-interacting systems, and we will therefore begin by implementing the modifications necessary to convert standard finite-element programs to include the stress/orientation distribution functions in the dilute and sporadic interaction ranges, with the expectation that this experience will be applicable to the

substantially-interacting systems when we are better able to understand their rheology in terms of structure buildup and destruction.

Block Copolymers (Williams/Spontak - GSRA). The ultimate goal of the research is to relate the mechanical properties of the block copolymer to molecular structure and such variables as temperature, block composition, and (when solvents are involved) to polymer concentration and polymer/solvent compatibility. In this last regard, there is a close connection to the research in polymer-solvent-nonsolvent thermodynamics and kinetics.

We plan to study the thermodynamics of phase separation in order to deal with the current inability to predict non-symmetrical interphase composition and interblock mingling. While some of these features may be manifestations of kinetic effects in sample preparation, such an explanation becomes less appealing when the small diffusion lengths and chain mobilities in the liquid state are considered. A new theoretical development of the overall system free energy is needed, with sufficient degrees of freedom allowed to permit these unexpected physical states to emerge as optimal. It is likely that the statistical mechanics of confined chains, a science now being developed, will have to be invoked.

Solvated systems need special emphasis. Only in the limit of "nearly neutral solvents" (those almost equally good for blocks A and B) is the microphase separation theory in satisfactory agreement with observations. The preferential solvent systems, which are of practical importance, need to be examined more closely. It is likely that appeals to colloidal nucleation theory can be combined with the existing theoretical framework to make progress here.

Experimental work in this area will utilize microscopy and rheology. The morphology in the normal solid state (and in the liquid state, trapped by a

rapid quench) can be examined by transmission electron microscopy (TEM) and--if facilities permit--also by SAXS. Indirect measurements, by tracking G'(T) and G"(T) with a torsion pendulum (solids) or Weissenberg rheogoniometer (liquids), are especially helpful for identifying transitions and are sensitive to minute details of microstructure.

The phenomena that need explanation in the liquid-phase rheology include yield stresses, unusually-strong viscous shear thinning, and some evidence of multiple stable or metastable states under steady shear-flow conditions. Theoretical approaches to explaining this behavior will involve a sequence of modeling fluid states of increasing disorder. At the lowest level is the highly ordered array of liquid domains at rest; shear in such a system causes deformation but not necessarily flow (i.e., a yield stress should appear) as long as molecular tension is unable to overcome thermodynamic demixing forces encountered by a block being pulled through its interphase. Theoretical estimates of maximum possible yield stresses should be achievable by summing over all such chains. (Reductions from these values should arise from "chunk breakage", as flow initiates with the localized partial disruption of the structure.) Thermodynamics couples strongly with the rheology here, through the demixing force barriers and the strain energy in the deformed network.

Non-Newtonian flow and some aspects of the multiple-state problem can also be treated by describing the thermodynamic state of the system in shear. Altered domains--smaller as chains disengage, and also deformed in the shear field--must be modelled realistically. It is likely that anomalous strain energy will again be a major new factor in the thermodynamic balance, with the possibility that true homogenization could occur at sufficiently high shear rates. (This behavior is in fact characteristic of domain behavior in polymer liquid crystals that are not formed from block copolymers, and similar

analytical procedures might be applicable in both classes of materials.) If "chunk flow" occurs, the modeling will have to be shifted to localized conditions near the edge of the chunk.

Experimental rheology will employ a newly-developed yield-stress measuring device that controls the imposed stress in a simple-shear configuration, cone-and-plate and parallel-plate torsional flows in the rheogoniometer for steady viscosity and elastic normal stress measurements, and the same rheogoniometer geometries in characterization of small-amplitude oscillatory response. For the latter case, we see a major need to vary the strain amplitude until the microstructure approaches failure; preliminary evidence indicates a surprisingly-large degree of strain-sensitivity in these properties. Ultimately, the critical connection between flowing microstructure and macroscopic properties will have to be made by optical methods that are not yet available in our laboratories.

Polymer-Solvent-Nonsolvent Interactions (Soong/Caneba - GSRA). The generation of asymmetric membranes for a binary system involves casting a homogeneous polymer solution between parallel solid surfaces, followed by application of a low temperature at one face of the cast solution. Since the theory of phase separation kinetics is already developed for metal alloy binary systems, it will first be extended to polymer/solvent binary systems before adaptation to ternary systems. At each stage, experiments will be performed to determine phase separation kinetics and composition of the phases, and to evaluate parameters needed for computer modeling. Predictions of porosity profiles of the final membranes will be checked by electron microscopy.

Flory-Huggins theory with concentration- and temperature-dependent χ-parameters will be employed for the thermodynamic relationships needed for the binodal and spinodal curves and for the terms involving free energy in the

spinodal decomposition diffusion equation. For the mobilities of the different components in the system, a free-volume expression will be adopted; i.e., a concentration-independent (but temperature-dependent) front factor multiplied by a concentration-dependent exponential term. For the mobility of the polymer at high concentrations, scaling concepts by de Gennes (based on reptation theory) will be employed. For coagulation of the cast polymer solution, we will consider both spinodal decomposition and nucleation and growth as possible phase separation mechanisms. We will refine the fundamental approaches used in metallurgy to understand the physics and mathematics behind these phase separation processes.

The binodal and spinodal curves in the phase diagrams will be determined through light scattering and pulsed NMR experiments. For the initial stages of spinodal decomposition (where the linearized form of the spinodal decomposition diffusion equation is applicable), light scattering experiments will provide values of model parameters at the overall concentration and temperature of the mixture. To obtain the coexisting phase compositions in the polymer solution, proton-FTNMR and ^{13}C NMR (with 180°-τ-90° pulse sequence) can be employed. With proton-FTNMR, we need to use a mixture of deuterated and undeuterated solvent to suppress the overwhelming solvent peak in the spectrum. We will also investigate the feasibility of obtaining kinetic information for the mobilities, gradient energy coefficients and concentration profiles in our phase separation model.

Discretization techniques will be used to model the transport of heat (for the binary system) or mass (for the ternary system) in the cast solution. Within the discrete units, de Fontaine's diffusion equation using periodic boundary conditions will be solved in one dimension. The nonlocal transport coefficients are then determined by a combination of calculated

local transport coefficients along the directions parallel and perpendicular to the concentration profiles at a particular slice of membrane material. The overall solution scheme for structure formation in the membrane would be to solve first for the concentration profiles assuming no change of state within the membrane. Then membrane structure can be determined from the phase separation diffusion equation. With this membrane structure, the previously calculated concentration profile can be corrected. The procedure is iterated until convergence.

Co-Processing (Denn/van de Griend-GSRA). We will study the interface development between two immiscible liquids in co-current flow, both experimentally and using finite-element numerical methods. The experimental work will employ the new laser speckle method of velocity determination, with a need to extend the procedure to deal with the presence of a fluid-fluid interface. The standard finite-element programs currently available for polymer fluid flow will similarly need to be modified to allow for the presence of the interface at an unknown surface in the flow geometry.

Co-injection molding is a transient process, in which the skin fluid is first metered into the mold, and is then displaced and moved to the mold walls by the injection of the (usually higher viscosity) core fluid. We will begin our studies with the easier problem of steady co-current flow, which is relevant only to the region behind the advancing front. The numerical work will begin with flow in a straight channel for program-development purposes, and we will then study the steady-state interface location in the neighborhood of a 270° angle, with fully-developed flow up-and downstream. The initial computation will be for immiscible Newtonian and power-law fluids, followed by computation for simple viscoelastic models.

Similarly, we will use steady co-current flow of Newton fluids in a

straight channel as the flow field with which we develop the experimental procedure, after which we will turn to steady co-current flow between fully-developed regions connected by a sudden contraction and a 90° sharp bend.

Molecular Weight Distribution Control (Soong/Denn/Freeman - GSRA). We plan to develop a mechanistic model of copolymerization kinetics that includes the gel effect and the concomitant concentration dependence of the monomer reactivities, to be coordinated with an experimental study of the kinetics and model validity in a continuous flow stirred reactor. The kinetic model will be used to study the effect of reactor configuration on operability, with the expectation of using control-theoretic methods to define satisfactory operating programs.

Partial Facilities List, UC Berkeley Polymer Laboratories

1. Rheometrics Mechanical Spectrometer 705-M.
2. Weissenber Rheogoniometer R-17.
3. Instron Capillary Rheometer, rated at 400°C and 15,000 p.s.i.g.
4. Five-ton Instron closed-loop servo-hydraulic test system with external computer control, capable of high-speed experimentation (20 in/sec plunger speed at 7,000 lb. load).
5. Ten-ton MTS servo-hydraulic test system with controller, signal generator, video display and recorder, and environmental chamber.
6. Rheo-Vibron Model DDV-II-B, and an equivalent instrument fabricated here having improved temperature and mechanical characteristics with on-line data processing.
7. Perkin-Elmer Differential Scanning Calorimeter DSC-2.
8. Laser light transmission unit, fabricated here. Designated to detect thermal transitions which generate microstructure from 25°C-300°C.
9. Torsion pendulum, fabricated here, with on-line data analysis.

MORTON M. DENN

B.S.E (high honors), Princeton University, 1961, Chemical Engineering
Ph. D., University of Minnesota, 1964, Chemical Engineering
Postdoctoral Fellow, University of Delaware, 1964-65, Chemical Engineering

University of Delaware:

Assistant Professor, Chemical Engineering and Statistics and Computer Science, 1965-68
Associate Professor, Chemical Engineering, 1968-71
Professor, Chemical Engineering, 1971-77
Acting Chairman, Department of Chemical Engineering, January-June, 1975
Allan P. Coburn Professor, 1977-81

University of California, Berkeley:

Professor of Chemical Engineering, 1981-

Visiting Positions:

Massachusetts Institute of Technology, Department of Chemical Engineering, Visiting Lecturer, 1978-
University of Delaware, Department of Chemical Engineering, Adjunct Professor, 1981-83.
Sydney University, Australia, Visiting Professor, May-June, 1976.
Monash University, Australia, Visiting Professor, May-June, 1978, 1979.
National Chemical Laboratory, Poona, India, U.S. -India Exchance of Scientists Program, March, 1979.
Technion-Israel Institute of Technology, Fulbright Lecturer and Harry Pierce Professor, September, 1979-January, 1980.
California Institute of Technology, Chevron Energy Professor, February-July, 1980.

Honors:

Guggenheim Fellow, 1971-72
Professional Progress Award in Chemical Engineering, 1977, from the American Institute of Chemical Engineers "for his incisive investigations into polymer processing and his pioneering studies into process dynamics and control"
William N. Lacey Lectureship, California Institute of Technology, 1979
Fulbright Lecturer, 1979-80
Peter C. Reilly Lectureship, Notre Dame University, 1980

Major Professional Activities:

Trustee, CACHE Corporation, 1982-
Editorial Board, Journal of Non-Newtonian Fluid Mechanics, 1976-
Editorial Board, The Chemical Engineering Journal, 1978-
National Center of Intermedia Transport Reasearch, Science Advisory Committee, 1983-
Engineering Foundation Conferences Committee, 1979-81
American Institute of Chemical Engineers: Awards Committee, 1978-; Subcommittee on Process Dynamics and Control of National Program Committee; Ad Hoc Accreditation Visitor.
Program Chairman, 1974 Joint Automatic Control Conference
Co-organizer and Co-chairman, Engineering Foundation Conference on Chemical Process Control, 1976
American Automatic Control Council: Technical Committee on Energy and Power Systems, 1982-
Member, American Institute of Chemical Engineers, Society of Rheology (U.S.), British Society of Rheology, Sigma Xi

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EDUCATION:

University of California, Berkeley
Chemical Engineering, Ph.D. (1978)

University of California, Berkeley
Chemical Engineering, M.S. (1977)

National Taiwan University
Chemistry, B.S. (1973)

HONORS: Earl C. Anthony Fellowship
1976-77

EXPERIENCE:

1975-78	Teaching/Research Assistant Department of Chemical Engineering University of California Berkeley, California
1978-1979	Post-doctoral Research Associate Department of Chemical Engineering University of California Berkeley, California
1979-1983	Assistant Professor Department of Chemical Engineering University of California Berkeley, California
1983-pres	Associate Professor Department of Chemical Engineering University of California Berkeley, California

PROFESSIONAL ASSOCIATIONS:

Polymer Division, American Chemical Society

American Institute of Chemical Engineers

Society of Rheology

Sigma Xi

SOCIETY ACTIVITIES:

Membership Committee, Polymer Division, American Chemical Society

Polymer Examination Committee, Polymer Division, American Chemical Society

Board of Directors, Golden Gate Chapter, Society of Plastics Engineers

Editorial Advisory Board of Journal of Applied Polymer Science

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EDUCATION

Ph.D. in Chemistry, California Institute of Technology, October 1980.
Adviser: Prof. Robert W. Vaughan (deceased, May 25, 1979);
Prof. Sunney I. Chan
Thesis: The Development of Novel Nuclear Magnetic Resonance Techniques for the Study of Solids, Thin Films and Surfaces with Particular Application to Amorphous Semiconducting Silicon-Hydrogen Films

B.S. in Chemistry, University of California, Santa Barbara, June 1976.

EMPLOYMENT

Assistant Professor, Dept. of Chemical Engineering, University of California, Berkeley, September 1982 - Present
Postdoctoral Fellow, IBM T. J. Watson Research Center, November 1980 - August 1982
Teaching Assistant, California Instititute of Technology, Fall 1976, Spring 1978, Winter 1979
Research Associate, University of California, Santa Barbara, June 1974 - August 1976

HONORS

Invited speaker at the 1981 March Meeting of the American Physical Society
Invited speaker at the 9th International Conference on Liquid & Amorphous Semiconductors, 1981
1981 Outstanding Young Men of America
Awardee: National Science Foundation Energy Related Fellowship, 1977-79
Dean's List Scholar, graduate with honors, University of California, Santa Barbara
Participant: National Science Foundation Research Program, 1975 and 1976
First Place Prize for presentation of original research, Student Affiliate ACS meeting, University of Southern California, 1976
Awardee: President's Undergraduate Research Fellowship, 1975 and 1976
Awardee: California State Scholarship, 1972-1976
High School graduate with honors

PROFESSIONAL SOCIETY MEMBERSHIPS

American Association for the Advancement of Science
American Chemical Society
American Institute of Chemical Engineers
American Physical Society

MICHAEL C. WILLIAMS

Biographical Information

Personal. Born June 11, 1937. Married, four children.

Education

B.S. (ChE), University of Wisconsin - Madison, 1959.
M.S. (ChE), University of Wisconsin - Madison, 1960.
Ph.D. (ChE), University of Wisconsin - Madison, 1964.

Student Honors

Allis Chalmers Scholar, 4 years (undergraduate).
Sophomore and Senior High Honors, University of Wisconsin.
Honorary societies: Tau Beta Pi (chapter vice-president), Phi Lambda Upsilon, Phi Eta Sigma.
National Science Foundation Cooperative Fellow, 4 years.
NSF Postdoctoral Fellow (declined in favor of different offer).

Experience

Professor of Chemical Engineering, University of California, Berkeley (1972--); Associate Professor (1968-72); Assistant Professor (1965-68).
Postdoctoral Fellow, Institute of Theoretical Science, University of Oregon, Eugene (studied the theory of polymer solutions, under M. Fixman), 1964-65.
Thesis research, "Normal Stresses and Related Viscoelastic Phenomena in Polymer Solutions," under R. B. Bird, 1960-64.
Research Assistant, Polychemicals Department. E. I. duPont de Nemours & Co., Wilmington, Delaware (flow instability with viscoelastic materials), summer 1961.
Research Assistant, K Division, Los Alamos Scientific Laboratory, Los Alamos, New Mexico (rheology of uranium suspensions), summer 1960.

Professional Societies

Society of Rheology.
American Institute of Chemical Engineers. (Materials Division)
American Chemical Society. (Polymer Division)
American Society for Engineering Education.

Publications

The total number of research papers in print or in press is 90; three reviews of books on rheology and two non-research articles have also appeared.

Pub-5106

WORKSHOP ON CAM PROGRAM ON METAL COMPOUNDS AS CATALYSTS

October 27–28, 1983

Lawrence Berkeley Laboratory

Co-Chairmen

G. Somorjai
H. Heinemann

Panel Chairmen

R. Levy (Catalytica Associates)
J. Norton (Colorado State University)
J. Rabo (Union Carbide Corporation)

October 1983

Lawrence Berkeley Laboratory
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This work was supported by the U.S. Department of Energy
under Contract No. DE-AC03-76SF00098

Contents

Introduction 1
Organization and Proceedings of the Workshop 1

Panel Discussions and Conclusions 3
Policy Recommendations 3
Specific Recommendations 3

APPENDIXES

A. List of Attendees A-1

B. Agenda B-1

C. Prepared Comments by Attendees C-1
Zeolites C-1
Comments on Transition Metal Compounds Presentation C-2
Novel Materials in Catalysis C-5

D-1 Questionnaire D-1

D-2 Evaluation of Questionnaires Handed Out at Workshop on Catalysis Program D-2

E. Panel Participants E-1

F-1 Panel 1 -- Zeolites F-1
Policy Recommendations F-1
Program Recommendations F-1

F-2 Panel 2 -- Transition Metal Compounds F-2
General Comments about CAM Program F-2
Choice of Materials for the Transition Metals Program F-2
Focus of the Program F-3

F-3 Novel Materials in Catalysis F-4
General Comments F-4
Technical Comments F-4

40-574 O - 85 - 90

G. Discussion Document for the CAM Program on Metal Compounds as Catalysts G-1
Metal Compounds as Catalysts G-1
Research On Zeolites G-2
Background G-2
Proposal G-3
Relationship of Synthesis and Structure G-3
Novel Zeolite Catalysts G-5
Literature References G-8
Studies of Transition Metal Compound Catalysts G-10
Background G-10
Proposal G-12
Literature References G-13
Novel Materials in Catalysis G-15
Background G-15
Proposal G-15
Organic and Organometallic Chemistry on Surfaces G-15
Novel Polymers G-19
Novel Electrodes in Electrocatalysis G-21
Literature References G-23
Personnel G-26
Interaction with Industry G-27

Introduction

A workshop was held on October 27th and 28th, 1983, at the auditorium in Bldg. 50 at LBL, to review a discussion document which had been submitted to the attendees. This document is contained in Appendix G of this report. Thirty-five invited attendees from industry, universities, and other national laboratories attended the meeting. An attendance list is given in Appendix A. The chemical, petroleum, and petrochemical industries as well as catalysts manufacturers were well represented. Industrial attendees came from both large and small companies.

It was the major purpose of the workshop to get comments, suggestions, and evaluations of the proposed program, and to obtain opinions on the program's potential value to industry. The results of the workshop as summarized in this report, fulfill the objectives set for it.

Organization and Proceedings of the Workshop

The agenda for the workshop is shown in Appendix B. The workshop was organized to allow presentation by various prospective investigators on their ideas and programs for the CAM catalysis program. The three projects in the program, "Zeolites," "Transition Metal Compounds," and "Novel Catalysts" each were presented by two to five investigators who added considerably to the content of the discussion document. After each series of presentations for each of the projects, two or three invited attendees commented on the presentations and the document. Some of these official comments are in Appendix C.

Prior to these sessions and in his introductory remarks, Professor Somorjai presented a charge to the attendees, and a questionnaire was distributed (Appendix D). This questionnaire was filled in by a majority of the attendees after the meeting. Brief abstracts of their comments are also contained in Appendix D.

Following presentations by investigators and invited comments as well as some discussion, the attendees split into three panels, one each on the subjects of zeolites, transition metal compounds, and novel catalysts. Attendance in each of the panels is given in Appendix E. Each panel was chaired by a scientist of recognized accomplishment in the specific field. Dr. Jule Rabo of Union Carbide headed the zeolite panel, Dr. Ricardo Levy of Catalytica Associates, Inc., headed the transition metal compounds panel, and Dr. Jack Norton of Colorado State University was chairman of the novel catalysts panel. The panels were also participated in by the prospective investigators of the different projects. Following an almost full day of deliberations, the panels arrived at recommendations which are contained in Appendix F and which are summarized in the following section of this report. In general, the recommendations were positive and supportive. Several excellent suggestions were made.

Panel Discussions and Conclusions

The recommendations of the panels, which are given in detail in Appendix F, can be divided into policy recommendations and specific recommendations.

Policy Recommendations

1. CAM should carry out fundamental research in areas of broad interest to U.S. industry, focussed on advancing understanding rather than development of new products and processes.
2. Advances in relevant new science should be communicated to the scientific community on an ongoing basis.
3. A policy should be developed to assure the priority of communication to U.S. industry.
4. A policy should be established by DOE to ensure adequate protection of U.S. interests in new developments issuing from national laboratories funded by public monies. This policy should cover patents (world-wide) and personnel. Industrial fellows should be selected only from U.S. industry; CAM postdoctoral fellows should not have foreign industrial connections.
5. Initial goals of the first-year program of CAM should be limited in view of the limited initial funding, and to avoid too much diversification.
6. It will be necessary to increase the permanent LBL staff working on CAM projects so as not to depend totally on graduate students and postdocs, and to provide continuity. It was agreed that this could probably not be done within the fiscal constraints of the 1984 budget.

Specific Recommendations

Zeolite Program

a) Microporous crystalline materials such as zeolites and related materials are suitable subjects for research.
b) A long-range research program should be initiated, focussing on chemical and structural observations and characterization of the solution chemistry leading to nucleation and

growth of crystal phases. Appropriate techniques should be developed for observation of relevant phenomena.

c) Suitable additional areas of fundamental zeolite research are:
   - Develop advanced zeolite techniques and related instrumentation for the study of zeolites.
   - Characterize the chemical and physical properties of the intra-crystalline environment.
   - Characterize the nature of the bonding within zeolite crystals.
   - Theoretical crystal modeling.
   - Characterization of catalytically reactive sites.
   - Definition of dynamic pore size.
   - Study of defect structure.

Transition Metal Compounds

a) Study systems which are active under realistic conditions of industrial interest. The stability of the materials under industral operating conditions should be studied early in the program.
b) The research should concentrate on developing fundamental understanding of phenomena.
c) Focus should include synthesis of surfaces of specific compositions either through bulk or supported systems.

Novel Catalysts

a) The work should search for new catalytic materials that can catalyze new reactions. The research program should emphasize generic studies aimed at understanding the relationship between the adsorbate and the catalyst.
b) The electrochemical proposals are interesting but need further definition.

Appendix A. List of Attendees

CHEMICAL MATERIALS WORKSHOP

OCTOBER 27-28, 1983

LIST OF ATTENDEES

Dr. R. R. Chianelli (201) 474-0100
Exxon Research & Engineering Company
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P. O. Box 45
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Dr. Delbert H. Meyer (312) 420-5412
Director, Exploratory Research
Amoco Chemical Corporation
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Mapleville, IL 60540

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Catalysis Institute
Chemical Engineering Department
University of Delaware
Newark, DE 19711

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Department of Chemistry
Colorado State University
Fort Collins, CO 80523

Professor A. G. Oblad (801) 581-6647
Department of Fuels Engineering
University of Utah
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Dr. William O'Grady (516) 666-2829
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Vice President-Manager
Technical Department
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Louisville, KY 40232

Dr. Richard Sapienza (516) 282-6666
Department of Applied Science
Brookhaven National Laboratory
Upton, NY 11973

Dr. Julius Scherzer (213) 263-5111
Director, Materials Research
Filtrol Corporation
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Dr. George Shier (517) 636-1997
Laboratory Director
Dow Chemical
1712 Building
Midland, MI 48640

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Prepared 11-03-83

Appendix B. Agenda

CAM WORKSHOP ON METAL COMPOUNDS AS CATALYSTS

AGENDA

Auditorium, Building 50, LBL

THURSDAY, OCTOBER 27

8:00am	Bus Pickup - Hotel Durant
8:00 - 9:00	Registration
9:00 - 9:05	**WELCOME** - Gabor Somorjai, Program Director
9:05 - 9:10	LBL Overview - Earl Hyde, Deputy Director - LBL
9:10 - 9:25	CAM Overview - Kenneth Pitzer, Director - CAM
9:25 - 9:40	**INTRODUCTION - Catalysis Program** - Gabor Somorjai, Heinz Heinemann, Deputy Program Director
	Zeolite Presentation
9:40 - 9:50	Electronmicroscopy - Ronald Gronsky
9:50 - 10:00	Synthesis - Richard Anderson
10:00 - 10:10	NMR - Alex Pines
10:10 - 10:20	Organic Chemistry - Wilhelm Maier
10:20 - 10:35	**Coffee Break**
10:35 - 11:15	Comments on Zeolite Project - Howard Sherry, C.D. Prater, Robert Van Nordstrand
11:15 - 11:25	**Transition Metal Compounds Presentation** - Alexis Bell
11:25 - 11:35	Synthesis - Angelica Stacy
11:35 - 11:45	NMR - Jeffrey Reimer
11:35 - 11:45	Characterization - J.N. Michaels
12:00 - 1:30	**LUNCH - Cafeteria**
1:30 - 2:00	Comments on Transition Metal Compounds Presentation - Ricardo Levy, Andrew Kaldor, A.W. Sleight
2:00 - 2:15	**Novel Catalysts Presentation** - Peter Vollhardt
2:15 - 2:30	Electrocatalysis - Marcin Majda
2:30 - 2:45	Theory - Leo Falicov
2:45 - 3:10	Comments on Novel Catalysts Presentation - Jack Norton, William O'Grady
3:10 - 3:15	**Coffee Break**
3:15 - 4:30	Panel Discussions Group A - Zeolites - Auditorium - Chairman: Jule Rabo Group B - Transition Metal Compounds - Rm 50B Chairman: Ricardo Levy Group C - Novel Catalysts - Room 50D - Chairman: Jack Norton
6:10	Bus Pickup at Hotel Durant
6:30 - 9:00	**DINNER - Dr. Somorjai's Residence** 665 San Luis Road, Berkeley

FRIDAY, OCTOBER 28

8:30 am	Bus Pickup at Hotel Durant
9:00 - 11:45	Panel Discussions and Reports Preparation
12:00 - 1:30	**LUNCH - Cafeteria**
1:30 - 2:30	Report Presentation and Closing

Appendix C. Prepared Comments by Attendees

In the following, brief abstracts of comments by invited attendees are presented.

Zeolites

Comments by Dr. Howard Sherry, P.Q. Corporation:

Little is known about how to intentionally synthesize a theoretically-proposed structure or any other structure. Almost all zeolite synthesis is empirical and serendipical. The most fundamental problem in zeolite synthesis is to understand the species that form the nucleation and the species that grow on this nucleation site. It is a complex system. There is a polymeric system of aluminum oxide and silicon dioxide, as well as sodium oxide; there exists a whole equilibrium or non-equilibrium distribution of polymeric fragments, ranging from monomers as a function of pH, temperature, concentration and other variables. The solution chemistry should play a very key role in the research program. When we finally know what species are the building blocks of the nuclei and/or of the crystals, and what values of temperature, pressure and compositional variables are necessary to allow the desired alumina silicate species form, then we will know what species lead to what zeolites.

Once you have learned to control the formation of species in solution, it should be possible to move to the next phase of the program, synthesis of zeolites that possess the hypothetical diffusional and catalytic properties you want to work with.

In the area of producing large crystals for surface studies, it is well to be aware that under the conditions at which one may synthesize these large crystals, different results may be obtained than if one produces small crystals.

In summary, the overall objectives of the program are to understand the fundamentals of zeolite crystallization. This information would then be used to synthesize theoretical zeolite structures, to synthesize structures based on the requirements of the catalytic process, to relate the crystal structure acidity and other physical/chemical properties to the catalytic properties; and finally, to introduce catalytically-active metals into known positions via framework substitution of tetra-hedral items or via interstitial substitution of cations or salt molecules into the pores of zeolites. The accomplishment of a program like this would be a tremendous contribution to both the science of catalysis and to technology. While some of us have tackled bits and pieces of it over the years, we have not gotten very far with it. I believe that this institution certainly has the strengths to do this kind of program.

Dr. C.D. Prater, California Institute of Technology:

This program, in which we are very interested, constitutes a sort of bridge between the academic and the industrial types of research; it holds very great promise. A part of the program that interests me a great deal is the one on trying to understand the way zeolite structures come about, namely, the synthesis. There are a number of trouble spots, however, that ought to be pointed out. You will probably have trouble acquiring and maintaining the art in zeolite synthesis. It has been a largely empirical approach, but there is a wealth of art in it. You will have to acquire at least some of this art and maintain it, and with having a graduate student and postdoctoral program, this may become somewhat difficult. You need to maintain the art while you try to put a scientific foundation under it.

This is a very rich program, in general, and even though it is fairly well focussed, there is, I believe, more than you can do with the people you have and with the limited resources. You may have to cut down on some things and concentrate more heavily on other things.

Concerning a later possible expansion of the program, you have all the proved techniques that we have heard so much of and know about. A problem that has been neglected is aging or the state of the catalyst as it is actually seen in the industrial environment. Most of the studies that have been done in academia and also, to a great extent, in industry have been concentrating on what one might call "start of cycle activity." This activity does not last for a very long time. The catalyst changes that occur, the reasons for aging, the sites involved, and physical changes in the structure should be investigated.

Dr. Robert Van Nordstrand, Chevron Research Corp.:

Past efforts to synthesize zeolites have been like pass, punt, and pray. You seal solutions in a teflon container; you heat; and you pray that something will come out. What we need in synthesis is understanding. Call it art, if you want to, but we need understanding of the art. We need to know what goes on in the teflon reactor. The alumina concentration changes, silica species change, templates concentration is important. Perhaps even the chemistry of the template changes as do the surroundings of the template, conductivity, viscosity, etc. All of these change and influence strongly what is going on. Once we understand what happens in the reactor, we need to assume control. Here is where I think the great instrumentation capabilities and the understanding of the theory of solutions provide ideal leadership in Berkeley. Hydrophobic interactions with solutions, for example, has been studied here, and is an integral part, in my opinion, of the zeolite synthesis, particularly the high silica synthesis. The great advances in electron microscopy, electron diffraction, etc., have been alluded to. We can now see much more from electron diffraction than we did with classical x-ray diffraction. The relationship of synthesis to structure is worth studying and hopefully, five years down the road, may provide an important transition to actual catalysis.

Comment on Transition Metal Compounds Presentation

Comments by Dr. Ricardo Levy, Catalytica Associates, Inc.

I'll make my remarks relatively brief because there are several other people that I'm sure are going to add to what I have to say.

I think the area of transition metal compounds such as carbides, nitrides, and the other compounds that are the subject of this group of research programs has a number of advantages

as a choice for the CAM program, and I believe they provide an opportunity to maximize and demonstrate the skills of this laboratory. Why do I say this? The compounds have been known for quite some time, as all of you know. Yet there haven't really been any demonstrated important industrial breakthroughs or applications. They offer opportunities for development. What's most exciting is that these materials exhibit a broad range of physico-chemical properties which, coupled with the hints of unique catalytic behavior, and I use the word "hints" advisedly, do provide an opportunity to establish a scientific base from which industry can build. In this respect I believe that the programs that we heard this morning are directionally quite promising. I do want to provide some comments, though, and some suggestions. Foremost, I would urge the researchers to avoid rushing to discover the new platinum substitute. I think this is very good for purposes of obtaining funds, and obviously ultimately it's a wonderful goal. But it should not really be the key motivating force of these research groups or else I think they are not going to get too far. Instead I urge the group to emphasize the opportunity that this system offers to learn about some bulk and surface properties which in fact may be very important in catalysis. Second, I think the loop between characterization, synthesis and catalyst testing has to be very tight. This is one of the interesting features of this particular program but it will only work if those three or four key experimentalists that are going to lead the groups work very closely together. In this respect, I feel there is one area, or one element, of a loop that really hasn't been emphasized sufficiently in terms of taking advantage of these materials. And in a loose way I've called that theoretical interpretation, and what I'm taking about is the concepts of electron flow—whether it goes from the metal to the non-metal—concepts of d-bands, etc. And this is an area in which with my limited exposure to the Lawrence Berkeley Labs, I have a feeling they have great strength. In fact, what I see is the interface between characterization catalysis and theoretical interpretation being fed by the synthesis effort. Now, no sooner have I said that I see a greater need for theoretical effort here, I believe there is a tendency in the programs I heard on carbides, nitrides, and also on zeolites, for the effort to be spreading itself too thin. I urge the key project leaders and the directors to really step back and assess where the strengths are and maybe refocus their efforts. And if I may offer a suggestion—I think that the greatest strength that you offer is really in characterization with state of the art tools. Many of the spectroscopies, the nuclear magnetic resonance work, and so on, that we heard could well be a cornerstone for a lot of the work. And so if I had to make a choice, I certainly would emphasize this one, and have the catalysis, the theoretical interpretation, and the synthesis really feed this.

Comments by Dr. Andrew Kaldor, Exxon Res. & Eng. Co.

I have a suspicious feeling that we can probably save some time because almost everything that I was going to say has been said by Ricardo Levy.

After being involved with a previous group that came down here for a workshop on industrial involvement in catalysis, one of the recommendations that we had made at the time was that you in fact bring together a group from industry to perhaps define for you some of the objectives, rather than a situation where the industrial people are listening to your particular desires, interests, and so forth. I think that it's essential and necessary to do what you're doing now, which is to, in a sense, tell us what it is that you are interested in, get people acquaninted with your capabilities and expertise. But I think the next step has to be to try to get industry to define for you some of the key issues in the areas that you are interested in where they see scientific long range problems and projects. I think the opportunities are best if you move into

new areas in the materials sense and I think the transition metal compound program is characteristic of the kind of areas that are well worth pursuing. I have also noted a deficiency on theory in your plans. I see a tremendous opportunity for you to work on this side of the line and I really see a situation where industry has to take a role on the other side of the line. And one begins to look at this characterization-material synthesis-theory level-reaction studies, as a whole entity. All of us from industry, I think, encourage the characterization aspects of the program, the development of new techniques, new capabilities, addressing issues. There I think you can find a tremendous bridge to most industrial organizations. Theory and model reaction studies probably fit into the same category. When you begin to enter the materials area, that, in many ways, I view as our bread and butter in some sense. That's where our proprietary positions in many cases are defined. That's where the greatest area of sensitivity and concern is. That doesn't mean you shouldn't be in it, but it means that crossing the bridge into that area is where I see the greatest difficulty. Probably, what we much prefer is activities in a lab like this that are more generic in character, that outline general materials behaviors, that provide some fundamental insight into how materials behave under exposure to chemical environments.

Comments by Dr. A.W. Sleight, E.I. du Pont de Nemours & Co.

From a national or industrial point of view I think it's clear that in the area of catalysis the goals are new catalysts, new improved catalysts and new catalytic chemistry. The question is what are the various roles of the university, CAM, and industry. Basically I believe it is the university's role to train students and provide us with understanding. I think that one role that I have heard overemphasized a bit today has been that of providing new materials, new catalytic materials. There is always room for new catalytic materials but there are some misconceptions in that area. Basically, providing understanding will lead very naturally to new materials and new catalytic chemistry. I'm sure there are many of us here who have heard people tell us that all catalysis has been generated by empirical means and that the understanding has yet to do us much good. Nevertheless the empiricism is steadily growing more enlightened and the effect is real today and will become increasingly important.

One could take the view that metals, oxides, and sulfides are the bulk of the catalysts used in the world and that perhaps the reason for that is that nobody has bothered to look much at other materials. I think to take that view is really naive. In important areas of catalysis one would find very frequently that hundreds of different compositions have been patented. Many times they are very different compositions. But you can be sure that for every material that ends up being patented, an industrial lab has looked at hundreds of others which have never been patented because they were not any good. And this would include essentially the whole range of even the most esoteric sort of compounds that are around. By and large, the reason that we end up with oxides, sulfides, and metals as catalysts is simply because they are the stable materials.

I want to move briefly to a totally different area that has not come up here at all so far, but I think should be seriously considered. Many important catalysts are not single phase materials and there are synergistic effects which abound throughout, whether it's oxides, sulfides, or metal systems. These can be exceedingly dramatic and as yet no one would be able to predict, in many cases, that one would get totally different catalytic properties by combining two materials where the catalytic properties are already well known but the combination just yields something totally different. Microstructure in these cases becomes all important. You have good facilities here for getting at microstructure which could be applied to two phase systems. And I think a

rational approach to understanding synergism and multiphase kind of catalyst is something that you might consider undertaking. There's a need to study microstructure. In many cases, catalysts are improved not by changing anything in the composition, but simply by changing microstructure. Study the microstructures, relate them to catalytic properties, and then relate that to the synthesis variables. The questions of new materials as catalysts has already been brought up. Are you looking at new catalysts or are you really looking at a new catalyst precursor? Even if what you're doing is looking at a new catalyst precursor, not a new catalyst, that's fine as long a that's really all taken into account and this catalyst is well characterized after as well as before it goes into the reactor. Finally, I would question whether carbides or nitrides really are a good place to focus. As Ricardo Levy has mentioned, they are not important catalytic materials. I believe there are many other areas that we could define where we have important catalytic properties which we do not understand and where a lot of understanding could be brought to bear without your stepping on the toes of any of the industrial parties that happened to have already been working on those catalysts. So in summary, then, I would focus on the understanding in all of these areas and have the faith that that understanding will lead to better catalysts and new catalytic processes ultimately, as we begin to understand the relationship between surface chemistry and catalysis.

Novel Materials in Catalysis

Comments by Dr. J. Norton, Colorado State University

In evaluating the potential utility of electrocatalytic cycles of the type formulated in the first part of the proposal it is important to keep thermodynamic considerations in mind. Although, in principle, uphill reactions may be driven theoretically, such reactions are limited in their practical applications. There are possible relationships between organometallic chemistry and homogeneous catalysis inherent in this proposal which should be pointed out. For example, alkylidyne complexes of the type proposed in part 2 are known and have been extensively characterized on surfaces. They may be formed by reaction pathways which are related to homogeneous mechanisms. This kind of interplay between the exploration of organometallic and surface mechanisms may prove a useful aspect of this CAM program. The type of potentially conducting organometallic polymers proposed should clearly prove to be interesting materials. It might be possible to elaborate on these structures. Thus, starting from dimetallacyclobutanes or cyclobutenes, photochemical metal-metal bond cleavage would lead to the kind of odd electron species capable of polymerization. One can also imagine arriving at such novel materials by starting with mononuclear metal carbene or carbyne species, in a sense metallic analogs of ethylene and acetylene, and effecting their polymerization. The latter may proceed in either head-to-head or head-to-tail fashion. In the case of the carbynes cis- and trans-double bonds may form. Both of these approaches appear to constitute attractive ways of making metallic polymers.

Comments by Dr. W. O'Grady, Brookhaven National Laboratory

Part 3 of the proposal concerned with electrocatalysis has great potential in the area of the attachment of catalysts to conducting polymers and/or creating products in difficult-to-reach oxidation states. One of the important areas in this field is that of oxygen reduction.

Particular attention has to be paid to changes in the structure of the catalyst and the electrode surface in general as the reaction proceeds. Such changes may alter the mechanism of the process under investigation. Another worry is that of stability of substrates, products, and particularly deposited polymers during electrolysis. For example, hydrogen peroxide produced in the reduction of oxygen readily degrades polymeric thin films on electrodes.

Another important point relates to the proper design of an electrochemical cell. Frequently that design, because of mass transport and other problems, may be more important than the development of catalyst efficiency.

Finally, the redox chemistry of small organic molecules such as carbon monoxide and formic acid, would be a worthwhile target in the area of electrocatalysis. It should be possible to increase the operating voltage of, for example, the hydrogen cell (1.23 V). With the right kind of electrocatalyst, exciting applications in fuel cell technology might be possible.

Appendix D–1. Questionnaire

Please comment on the catalysis programs (zeolites, transition metal compounds, and novel catalyst preparation), and suggest ways of improving them.

Please suggest new long-range catalysis research programs that you consider important and appropriate for the CAM Catalysis effort.

New links to strengthen the academic-industrial interface through the CAM Catalysis Program are suggested. These are:

- Industrial Fellows
- Industrial Consultants
- Industrial Advisory Committee
- Joint Research Projects
- Industrial Users of SSCL Facilities
- Transfer of Personnel (temporary) to and from Industry
- Business Ventures (involving both CAM and industry personnel)

Please comment on these (appropriateness, probability of success) and recommend other ways to aid the linking of long-range research to technology.

Appendix D–2. Evaluation of Questionaires Handed Out at Workshop on Catalysis Program

Ninteen questionnaires were returned at the end of the meeting. The great majority of them raise and discuss points which were also brought out in the panel discussions, and which are summarized in the panel reports. In the following, certain comments are summarized which are not mentioned elsewhere and which were mentioned by more than one person.

The project entitled "Novel Catalysts" is considered by several people the weakest of the three projects, and one that needs considerably more focus and relationship to catalysis. This program needs much more development before a final judgement on its value can be made. It also appears to be of relatively little industrial interest.

A number of additional suggestions were made for new long-range catalysis programs. Among the most interesting is "Synergistic Effects in Heterogeneous Catalysis."

A repeated concern is the relatively large number of subjects in light of the low initial funding. It is felt that each of the three projects should concentrate on one or two major questions to start with and until additional funds become available. In this connection, it is repeatedly pointed out that the program may be too heavily concentrated on University personnel, and that more LBL staff personnel should be involved, respectively should be hired when funding permits continuity.

In the zeolite program, it has been suggested that a more generic approach to porous and layered materials should be considered, including zeolites. This is not essentially different from the recommendations of the panel.

The questions on the second page of the questionnaire, namely, "New links to strengthen academic-industrial interface through the CAM Catalysis Program" resulted in an overwhelming rejection of business ventures involving both CAM and industry personnel.

Industrial use of SSCL facilities is repeatedly recommended as a major plus. Industrial advisory committees and transfer of personnel to and from industry are also generally recommended. Industrial fellows appear desirable but it is foreseen that difficulties may arise in choosing the right people and getting companies' approval. Industrial consultants to CAM are considered of great value to the Laboratory but not necessarily to the companies. It also was pointed out that in addition to industrial fellows, there should be academic fellows from schools other than Berkeley.

Appendix E. Panel Participants

The attendees at the workshop were distributed between the different panels as follows:

Zeolites	Transition Metal Cmpds.	Novel Catalysts
Jule Rabo, Chairman	Ricardo Levy, Chairman	Jack Norton, Chairman
Carl J. Russ	R.R. Chianelli	Arturo Diaz
Julius Scherzer	John Gland	T. R. Hughes
Edith Flanigen	Andrew Kaldor	Ron Jensen
Alex G. Oblad	S.J. Lapporte	E.A. Mills
Alex Pines	Richard Sapienza	William O'Grady
Bob Van Nordstrand	H.J. Schoennagel	M.L. Poutsma
Tom Hughes	A.W. Sleight	Larry Schmidt
Wilhelm Maier	E. Wallace	John Sibert
John Ward	D. Meyer	Peter Vollhardt
Howard S. Sherry	Harvey Leadbetter	M. Majda
Charles D. Prater	Alex Bell	
Francis G. Dwyer	Angelica Stacy	
David Shaw	Jim Michaels	
Richard Andersen	Jeffrey Reimer	
Heinz Heinemann		
S. Mark Davis		

Appendix F–1. Panel 1—Zeolites
Jule A. Rabo, Chairman

Policy Recommendations

CAM should carry out fundamental research in areas of broad interest to U.S. industry, focussed on advancing understanding rather than the development of new products and processes.

Advances in relevant new science should be communicated to the scientific communitity on an ongoing basis.

A policy should be developed to assure the priority of communication to U.S. industry.

A policy should be established by DOE to insure adequate protection of U.S. interests in new development issuing from national laboratories funded by public monies. This policy should cover patents (world-wide) and personnel. CAM industrial fellows should be selected only from U.S. industry. CAM post-doctoral fellows should not have foreign industrial connections.

Program Recommendations

Microporous crystalline materials such as zeolites and related materials are suitable subjects for research.

A long-range research program should be initiated focussing on chemical and structural observations and characterization of the solution chemistry leading to nucleation and growth of crystal phases. Appropriate techniques should be developed for observation of relevant phenomena.

Suitable additional areas of fundamental zeolite research:

- Develop new advanced techniques and related instrumentation for the study of zeolites.
- Characterize the chemical and physical properties of the intra-crystalline environment.
- Characterize the nature of the bonding within zeolite crystals.
- Theoretical crystal modeling.
- Characterization of catalytically-active sites.
- Definition of dynamic pore size.
- Study of defect structure.

Appendix F-2. Panel 2—Transition Metal Compounds
R. Levy, Chairman

General Comments About CAM Program

It would be valuable for the groups to record the goals which they want to achieve in the *1st year*, particularly in view of the limited initial funding. Otherwise the expectations raised by the more ambitious goals of the whole program may lead to some short-term disappointments.

For the transition metal compounds project, cooperation among the project leaders and students is very important for the success of the effort. Awareness of the challenge inherent in this cooperation is also important.

From a global standpoint relating to the whole CAM program, there are other areas that should also be examined outside of catalysis, many which have surface related challenges such as high energy magnetic materials and H_2 storage materials.

Choice of Materials for the Transition Metal Compounds Program

Concern was expressed about the need to study systems which are active under realistic conditions of industrial interest. In this respect the chosen materials (carbides, nitrides, etc.) have not been proven. Specifically, the precedent for industrially-interesting catalytic activity is not nearly as extensive for C or N than, for example, other transition metal compounds such as sulfides and oxides. In view of this concern, if C, N, etc. are chosen, there should be a continuous awareness of the applicability of what is learned to other more "proven" systems. This also leads to a general comment that the researchers should review the advantages that C, N, etc. offer for the CAM program's short and long-term objectives, and assess whether other systems (such as oxides) may not meet these objectives as well. This does not means a unanimous recommendation to move to other materials. Many representatives support the general choice made by CAM for this program.

A specific aspect that should be addressed in the program is the stability of the materials under real industrial conditions, as well as their catalytic behavior. This should be done early in the program.

Focus of the Program

The research should concentrate on developing fundamental understanding of phenomena, and trust that industrial groups will use the information. It may be used in ways that neither the academic nor the industrial group anticipate.

Focus should include the synthesis of surfaces of specific compositions either through bulk or by supported systems. Such studies are likely to have many industrially-significant implications. In this respect, the development of new approaches and techniques of characterization should be emphasized.

Appendix F-3. Panel 3—Novel Materials in Catalysis
J. Norton, Chairman

General Comments

A unique role needs to be defined for CAM so that it will not merely duplicate existing university and industrial research. It should avoid the short-term (3 to 4 years, one "graduate student lifetime") approach necessarily characteristic of university research; it should involve permanent LBL members, and it should operate in a genuinely interdisciplinary way. CAM should also avoid the type of applied work that is best done in industrial laboratories; it should not just aim for increases in rate, etc., but should search for new materials that can catalyze new reactions. There are many advantages in having industrial laboratories assess the catalytic potential of new materials developed at CAM. The CAM research program should emphasize generic studies aimed at understanding the relationship between synthesis, structure, and reactivity. Acceptable mechanisms for commercialization of discoveries should be formulated early. Policies covering various legal situations (transfer of proprietary information in both directions, publications policies, and future development rights) must be established before interaction with industry can begin. These policies should be broad enough so that individual cases can be negotiated. Industrial fellowships and retraining programs at CAM should work well, particularly if the time period involved is flexible. Student internships and academic sabbaticals in industry should be encouraged. Such exchange of personnel is more worthwhile than the use of consultants. The advisory committee should include a broad cross-section of industry, should meet frequently, and should be kept well-informed on all activities at CAM. Industrial use of SSCL facilities should be encouraged.

Technical Comments

The Novel Catalysts program is aimed at the synthesis of novel monomers and polymers of unusual electronic and metallic makeup. It is expected that these materials will show unusual solid state properties, such as conductivity, and solution phase behavior, such as the potential to act as ligands to transition metals. This in turn might provide metal compounds with novel catalytic activity. Some of these systems will be investigated with respect to their potential as electron-transfer mediators on electrode surfaces and in electro-catalysis.

The proposal appears singularly focused on deposited and/or immobilized potential catalytic and electrocatalytic systems. Yet clearly, homogeneous organometallic catalysts or catalyst precursors to be activated in a variety of ways (not necessarily electrochemically) would also constitute suitable targets. These could possibly have dual functionality in oxidation-reduction cycles. With respect to the specific catalytic processes to be investigated, input from the applied industrial sphere should be sought. Similar input might be appropriate and desirable in parts 2 and 3 of the proposal where a polymer chemist might bring to bear his/her unique expertise.

The proposal, particularly in its first two sections, is of a probing exploratory kind. There are clearly possible important applications which span beyond the scope of catalysis but which encompass other areas of materials science. These involve organic and organometallic conductivity, potential applications in fuel-cell and battery construction, solar cells, electromagnetic interference shielding and other devices.

Part 3 of the proposal, particularly in conjunction with the innovative ideas in the first two parts will impact the area of modified electrodes. Serious consideration has to be given to: 1) mass (or ion) transport problems in thin films; 2) electrochemical reversibility of the redox centers; 3) chemical stability of the polymers. However, it is anticipated that the unique combination of synthetic and electrochemical capability will lead to significant advances in the field. Other fruitful areas which should be explored in this project include: 1) the oxidation of small organic molecules, such as CO, formic acid, and methanol; 2) stereo- and regiospecific organic transformations; and 3) the construction of shape- selective electro-catalytic assemblies.

Overall, it is felt that the proposed work has the type of exploratory and innovative character with potential long-term applications which should be the unique feature of a CAM program.

Future expansion into other areas of homogeneous and heterogeneous catalysis is recommended, such as cluster catalysis, inorganic and organometallic reaction mechanisms, enzyme catalysis, and other novel molecular assemblies.

Appendix G. Discussion Document for the CAM Program on Metal Compounds as Catalysts

INDEX

METAL COMPOUNDS AS CATALYSTS 1

I. RESEARCH ON ZEOLITES 2

A. Background 2

B. Proposal 3

1. Relationship of Synthesis and Structure 3

2. Novel Zeolite Catalysts 5

C. Literature References 8

II. STUDIES OF TRANSITION METAL COMPOUND CATALYSTS 10

A. Background 10

B. Proposal 12

C. Literature References 13

III. NOVEL MATERIALS IN CATALYSIS 15

A. Background 15

B. Proposal 15

1. Organic and Organometallic Chemistry on Surfaces 15

2. Novel Polymers 19

3. Novel Electrodes in Electrocatalysis 21

C. Literature References 23

IV. PERSONNEL 26

V. INTERACTION WITH INDUSTRY 27

METAL COMPOUNDS AS CATALYSTS

Metal compounds, such as metal oxides, nitrides, carbides, and metallo-organics, etc. as well as intermetallic compounds have found widespread applications as catalysts in industry. Many of the oxides exhibit strong acid/base characteristics, while other compounds have characteristics which may make them suitable as replacements for precious metals, and still others permit a type of molecular engineering based on diffusional characteristics. Additional exploration of such materials holds considerable promise for the identification of new catalysts with properties superior to those now available.

The relationship of synthesis and structure on the one hand and of structure and catalytic properties on the other is in many cases poorly, if at all, understood and the preparation of catalysts of this type which possess optimal activity and selectivity is largely an empirical art. With a better fundamental understanding it can be expected that a rational approach to produce specific structures would become possible, structures which in many cases can be modeled today on the basis of theory but which cannot be synthesized because of a lack of understanding of the effect of variables in the synthesis on final product.

The present proposal tries to obtain answers to several fundamental questions, an understanding of which would greatly extend the usefulness and applications of industrial catalysts. The metal compounds to be considered are: 1) alumino-silicates (zeolites), which constitute one of the largest classes of commercially-used catalysts; 2) transition-metal compound catalysts such as carbides, nitrides, silicides, sulfides and borides, some of which may be useful in replacing rare and expensive precious metals which are not indigenous to the United States; and 3) metallo-organic compounds of catalytic activity, which may be heterogenized and combined with other metal compounds to exert dual functions, and which may be particularly applicable in electro-chemistry.

For purposes of easier reading, the document is subdivided into three areas listed above. Background information on these specific metal compound types is given at the beginning of sections I, II, and III of this document. While there are overlaps and relationships between the proposed investigations of the three types of metal compound catalysts, it is expected that as work proceeds, results from each of the investigations will influence and orient research in the others.

The LBL/UCB investigators together with graduate students and industrial fellows working on this proposal will collaborate as a team, rather than as individuals following a narrow area only. Each member will be in frequent, if not constant, consultation with the other members of the team, and will be fully aware of the objectives and the progress made toward achieving them.

I. RESEARCH ON ZEOLITES

A. Background

Zeolites are crystalline alumino silicates which have been known for well over 100 years. They occur in nature but during the last 30 or 40 years many have been prepared synthetically. They were originally used for ion-exchange procedures, an application that is still in large use. Due to their uniform pore structure as crystals, they have also found large-scale application in selective adsorption, particularly of water. Zeolites as water adsorbents give extremely low dew-point gases. In recent years, zeolites have found very large-scale application in detergents as a replacement for phosphates.

A very large application of zeolites has developed as it has become apparent that zeolites are outstandingly good catalysts and catalyst carriers. Zeolites today constitute the largest single class of industrial catalysts; in volume, they are surpassed only by automotive emission catalysts. Since zeolites, because of their preparation method, are relatively expensive, their value exceeds that of almost all other catalysts and even approaches that of precious metal containing catalysts. In view of this, it is, of course, necessary to have long catalyst life, and to possess methods for easy regeneration of these zeolites. This, in turn, implies that the zeolites must have high thermal and hydrothermal stability.

There are today some 150 known synthetic zeolites which differ in crystallographic structure, and which possess different characteristics such as different pore size, different acidity, and different silica/alumia ratios. Even within the same crystallographic structure, it has in some cases been possible to vary the silica/alumina ratio of certain zeolites over a range of three or four orders of magnitude. The ultimate number of zeolites which could theoretically be produced is almost infinite. Structures of zeolites of potential interest can be modeled, but no method of snythesis is yet known. The catalytic activity of zeolites is most often based on acidity characteristics; in many cases, zeolites perform in acid-catalyzed reactions. The acidity is ascribed to the interaction of aluminum with oxygen and silicon atoms, and the defect structure imposed on the aluminum by surrounding silicon and oxygen bonds. Changes in the silica/alumina ratio will change the number of acid sites and can influence acid strength. Incorporation of other metals into zeolite cavities or, if possible, into the framework, adds further dimensions to catalytic applications, as does the crystallization of zeolites around organic templates.

The large commercial applications of zeolites as catalysts use synthetic zeolites almost exclusively. Synthetic zeolites have been prepared by many methods, and are usually produced under hydrothermal conditions. While specific conditions of solution ratios, pH, temperature, and pressure, among other variables are known to produce specific zeolites, this knowledge is purely empirical, and reasons for the formation of specific zeolites under specific conditions are not understood. Some specific zeolites are crystallized around organic compounds often containing quarternary carbon or nitrogen atoms. The organic material is burned out after crystallization of the zeolite.

In the 1960s, the discovery was made that what has become known as shape-selective zeolites could be produced. These materials have pore sizes which restrict the easy diffusion of certain molecules into the pores, and therefore, become selective to certain molecular shapes. The great amount of work performed, particularly in industry or applications, of zeolites and their structure is evidenced by about 6,000 publications and patents during the past twenty years. Only a very limited number of these (twenty or so) refer to the question of relationship of synthesis and structure. It is also important to realize that of the 150 or so synthetic zeolites known, only about eight have found large-scale industrial use. There is very limited knowledge of the relationship of zeolite synthesis and zeolite properties. There has been appreciable work by individual workers, both in the U.S. and abroad, on physical, chemical,

and crystallographic characterization of zeolites, but there has been no published, intensive investigation of specific zeolites by interdisciplinary teams to determine essential characteristics leading to a better understanding of the functioning of zeolites, as well as an understanding of the nucleation processes that, during synthesis, lead to specific zeolite structures. Such interdisciplinary investigation, as described in the following section, would result in the ability to synthesize known model structures of zeolites, and gain a clearer perception of what it is in different zeolites that controls their catalytic action. It would potentially lead to the synthesis of more effective and selective catalysts for specific applications. Tools are now available and are continually becoming available for improving recognition of specific properties, and should be applied in conjunction to pinpoint distinguishing features between different zeolites, and even between zeolites of the same structure, but different chemical composition and different catalytic and adsorptive properties. Table I presents some of the tools and their areas of use, which have been applied during the last 3-to-4 years.

TABLE 1

	METHOD	USE
1.	High resolution 29Si and 27Al NMR, magic spinning angle NMR.	a) Determination of tetrahedrally coordinated Al in zeolites. b) Existence of Al rich/poor aggregates in zeolite catalysis.
2.	High-resolution electron microscopy.	Direct observation of zeolite rings and pore structure. Evidence of intergrowth of different zeolites. Evidence of amorphous zeolites.

B. Proposal

1. Relationship of Synthesis and Structure

It is the purpose of this project to bring to bear an interdisciplinary approach on the relationship of zeolite synthesis to the character of the zeolites produced. An understanding of the effect of composition and crystallography on number of acid sites and acid strengths as well as on shape-selective properties, will contribute to the manufacture of new and better catalysts for a large variety of purposes. In addition, the study should eventually extend to new materials having potential shape-selective characteristics such as crystalline-aluminum phosphates, zinc titanates, and layered clays.

Theoretical considerations indicate that the existence of a very large number (hundreds) of stable zeolites is potentially possible. One can build models of potential zeolites. While the theoretical structure of some of these indicate that they may be of great interest for applications, we do not know how to synthesize them. It is, therefore,

essential to create a better scientific basis for their synthesis, and for the variables that cause different chemical and physical characteristics of zeolites as catalysts. It is not intended to carry out chemical reactions over the zeolites other than as needed for specific characterization. The purpose of this program is a better understanding of zeolites themselves. Synthesis of zeolites is largely a black art, and a major purpose of this program is to correlate synthesis with zeolite characteristics.

Objectives and Approaches

While it is the long-term objective of this proposal to learn how to produce specific zeolites of predicted structure and catalytic characteristics, it is expected that a number of years of interdisciplinary work will be required to achieve such results. In the first year of this project, at least two industrial scientists of renown in zeolite technology will assist NCAM staff in setting up a synthesis laboratory and in producing two or three known synthetic zeolites of differing issue. These known zeolites will be characterized by x-ray diffraction, electron microscopy, solid-state NMR, EXAFS, and adsorption studies. A systematic change will then be made in the synthesis, varying one variable such as solution concentration, pH, temperature and time of chrystallization, etc. at a time, and studying the resulting changes in zeolite structure and characteristics. Of great importance will be the nucleation stage at which crystallization starts. It has recently been shown that cases in which templates are used to crystallize zeolites, NMR permits the observation of these organic molecules during nucleation, and permits some conclusions of their roles in structure formation. These and other colloid chemistry methods will be pursued with the help of a colloid scientist to be added to the NCAM staff.

In the second year, the staff will attempt to produce new zeolites on the basis of what has been learned about the effect of synthesis variables on crystal structure. The major attempt will not be to synthesize a large number of zeolites on an empirical basis, but to begin to learn how certain structural characteristics can be developed during synthesis. Additional objectives in this and subsequent years will be:

a) To deposit metals into the pores of the zeolite and to anchor them in predetermined positions in the pores and/or cavities. It will also be attempted to substitute metals of catalytic properties for some of the aluminums in the framework, and to pursue the stability and catalytic characteristics of these materials.

b) To place emphasis, in the synthesis, on crystal growth, and to make some rather large crystals (e.g., of one millimeter size) for surface science studies. It is clear that structure and composition should be varied separately, and that composition should be varied within a given crystallographic structure.

c) To investigate whether shape selectivity of certain zeolites can be imposed on metal-catalyzed reactions. Diffusion of organic and inorganic molecules into and out of the zeolites will be investigated and the diffusion path delinated. Crystallization of zeolites in non-aqueous media is worthy of consideration as are questions on the thermal stability or instability of zeolites and the reasons for same. The effect of poisons on surface properties will be investigated.

d) To determine location and strengths of acidity, the effect of acid strength and number of acid sites on such different reactions as cracking, isomerization, alkylation, and hydrogen transfer. An attempt will be made to determine why certain high silica/alumina ratio zeolites still possess high acidity and whether such acidity is due to an uneven distribution of aluminum through the crystal. The role of acid/base relationship in zeolites and that of Lewis acids will be explored.

e) In the synthesis, emphasis will have to be placed on crystal growth, and it will be necessary to make some rather large crystals (e.g., of one millimeter size) for surface science studies. It is clear that structure and composition should be varied separately, and that composition should be varied within a given crystallographic structure.

f) On the theoretical side, the suggestion has been made that in the diffusion of organic molecules through zeolites, the zeolite acts as a strong solid electrolyte, interacting strongly with the polarizable molecules. This raises the question as to whether there are useful analogies to the theory of ionic conductivity which might be developed.

g) One can also consider using zeolites as supports for small embedded transition metal particles, i.e., using the cage structure to stabilize dispersed metal particles in the range 7-10 A.

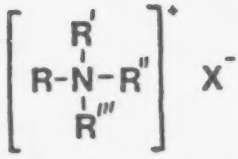
Many tools will be used to investigate the different preparations obtained. It will, for instance, be possible to compare ion scattering, which only investigates external surface, with ESCA which goes somewhat deeper and to complement this investigation with EXAFS and x-ray crystallography as well as electron microscopy. The combination of solid-state NMR and electron microscopy (shadowing techniques) provides a powerful method of structure identification. Recent work has shown the value of magic angle spinning NMR as a tool for determining the location of metal (e.g. A1 or B) and silicon atoms in the zeolite framework. This tool will complement the others. Adsorption studies will assist in defining diffusional properties of the zeolites. A new continuous catalytic testing unit, which is being installed at LBL during fiscal year 1983 ,will permit testing of new preparations for catalytic reactions.

Study of zeolite-metal particle systems could offer several interesting possibilities. First, in the making of such systems, one may consider the use of solid state channeling phenomena (i.e., particularly considering the natural channel structure of the zeolite itself), such as are used in ion implantation techniques for semiconductors. One may be able to control both composition and location of metal clusters. EXAFS may be used to infer the crystallographic siting of the particles and to study the metal-zeolite interactions. The whole array of modern surface physics theoretical and experimental technique for electronic structure can be used to study the charge transfer between metal and zeolite. XPS (x-ray photoemission spectroscopy) and associated theoretical calculation of electron structure should be valuable. Study of quantum size effects by susceptibility and NMR measurements should also be useful. Besides the electronic structure per se, one would want to study vibrational spectra, perhaps by Raman or neutron scattering, to see effects of the metal particles bonding to the zeolite internal surface.

2. Novel Zeolite Catalysts

a) *Synthesis of chiral shape-selective zeolites (inorganic enzymes).*

High crystallization rates and remarkable structure-directing effects by the use of tetra-propylammonium ions have especially been noted in type B ZSM-5 synthesis. Such structural effects by a binary organic cations offer a chance to synthesize chiral shape selective zeolites by the use of optically-active cations. The effect of optically-active ammonia ions, (a known, readily preparable, but little-investigated class of compounds) on zeolite synthesis will be studied.



R= aliphatic, aromatic, chiral

The chirality of the zeolites prepared will be studied by monitoring the optical rotation of product mixtures produced by simple reactions like the hydroisomerization of racemic 3-methyl-hexane. The detection of any optical induction will stimulate a limited optimization of the synthesis of optically active zeolites. Here, mainly crude effects will be studied: variation of Si/Al ratio, variation of chiral ammonium salt (chiral side chain and modifications in the relative steric bulk of the four different substitutents on the nitrogen atom). The most effective synthetic method as well as the most effective zeolite prepared will then be subject to intensive investigations (interdisciplinary investigation: relationship of synthesis and structure). The potential application of such chiral zeolites in all areas of zeolite catalysis and ion exchange reactions promises a wide field for investigations in the future.

b) *Modified zeolites with increased acidity*

One of the major areas of zeolite application is in the hydroisomerization of crude oil. This process is based on the cationic rearrangements of hydrocarbons catalyzed by acidic sites of zeolites. The objective of this project is to increase the catalytic isomerization properties of zeolites by framework or surface modifications.

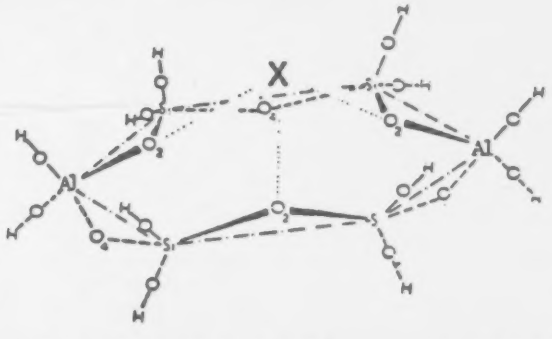
We propose the isomerization of endo-tricyclo[5.2.1.0] decane to adamantane as test reaction. This well-known isomerization reaction is not only very readily analyzed, but also very difficult to achieve under normal reaction conditions and therefore indicative of unusual catalytic properties.

In an unpublished investigation with a large variety of Lewis acids, it has been found that hafnium, zirconium, and titaniumchlorides were by far the most effective catalysts for this rearrangement process. The substitution of Si or Al atoms by these elements during zeolite synthesis as well as the effect of surface deposition of their chlorides will be investigated; the effect on isomerization properties will be studied. Modified zeolites, where other metals substitute aluminum or silicon in the framework, have been synthesized with only moderate success. Temperature dependent structural rearrangements seem to cause migration of atoms like boron and iron to the surface of the zeolite. Nevertheless, this area has not been thoroughly investigated yet and the catalytic potential of such framework modified zeolites more than justifies further investigations.

Successfully modified zeolites with improved catalytic properties (for rearrangement reactions) will be investigated thoroughly by the appropriate methods, especially with respect to the structural changes in the zeolite framework. Their structural stability as well as their reproducibility will be tested accordingly.

c) *Theoretical simulation of zeolite surfaces*

The increasing importance of zeolites in catalysis has led to the application of quantum mechanical methods. Of interest for us is especially the work of Beran, who used CNDO2 calculations to study the interaction of representative zeolite clusters with hydroxyl groups, and ethylene. Most promising is a recent publication in which he reports the inclusion of an electrostatic field in his calculations to represent the bulk zeolite crystal. We plan to calculate the interaction of zeolites with selected model substrates or metal atoms by a similar approach. The zeolites will be modeled as small $Si_mAl_nO_xX_yH_z$ clusters in a variable field of dipoles simulating the remote part of the solid. An example structure is depicted below. The dipoles, which will be located at the atomic positions of the next shell of remote Si, Al, and O atoms (x-ray structure), will be adjusted in size to force the complete geometry optimization of the "zeolite-unit" as close as possible to the experimental structure.

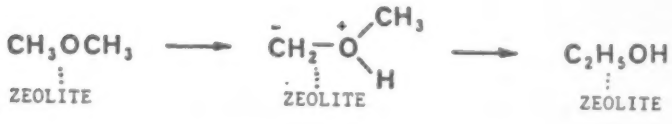


This procedure will provide 'unit cells' representing individual zeolites. These preoptimized 'unit cells' will be used to study physical and chemical properties of the zeolites as well as the interaction with substrates of interest.

Zeolites are especially well suited for such an investigation since its basic structures consist exclusively of Al, Si, H, and O atoms, which are well described by *ab initio* as well as semi-empirical quantum mechanical methods. The molecular size of even the simplest representative part of a zeolite structure, however, is prohibitively large for *ab initio* calculations; semi-empirical calculations are the only practical alternative at present. Especially the most recent development of MNDO, which includes d-orbitals for second row elements, should be well suited to provide a good quantum mechanical description of a zeolite surface. Furthermore, since MNDO has been parameterized to reproduce experimental properties this semi-empirical method seems to be most adequate for our approach. Initially we plan to study the gross effect of Si/Al ratio on the Bronsted acidity. We will calculate the proton affinity of the various positions of the zeolite unit and will thus not only locate the exact position of highest acidity but also determine the structure dependence of the acidity. Considering the overall excellent agreement of MNDO proton affinities with experimental results

we expect good agreement of our calculated numbers with experimental zeolite data.

After this initial study the computer generated zeolite models will be used to study and predict various features of interest. The effect of framework substitutions with other elements on structure and acidity, the location of hydrogen, sodium, or potassium atoms can be studied as well as the effect of the zeolite surface interactions on the reaction path of simple transformations like the conversion of dimethyl ether to ethanol.



Later we may also study the surface interaction of zeolites with transition elements of various oxidation states. These calculations may provide information about the interaction of zeolite surfaces with substrates, transition states, and products of catalyzed reactions. The results will be used to improve catalysts as well as reaction conditions and may lead to new catalyst modifications.

C. Literature References

The literature on zeolites contains many thousands of references. Only a small number of these pertain to synthesis, with the greatest proportion reporting reactions on zeolites. Another large number deals with structural determinations, and exchange of various ions into the pores, and varieties of zeolites, as well as adsorption and description data. Thus, a book dealing with a single application of zeolites (Venuto, P.B., and Habib, E.T., Jr., "Fluid Catalytic Cracking with Zeolite Catalysts," Marcel Dekker, Inc., New York, 1979) quotes 323 references.

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II. STUDIES OF TRANSITION METAL COMPOUND CATALYSTS

A. Background

Many of the metal catalysts currently used on a large scale are based on platinum, palladium, and rhodium. These noble metals are of strategic value and are not available in the U.S.[1] It would be highly desirable, therefore, to find replacements for these metals, or barring that, to find means for reducing the amount of noble metal needed to produce a viable catalyst. Among the materials which have shown promise in this connection are metal carbides and nitrides.[2,3] It is also quite possible that successful catalysts can be developed starting from metal silicides and borides, or from intermetallic compounds involving rare earth elements.

The primary goal of the project on metal compound and intermetallic catalysts will be the development of a fundamental understanding of the relationships between catalyst composition and structure, and catalyst performance. Through the use of a combination of physical techniques, the bulk and surface structures of the catalysts before and after use will be defined. The effects of reaction conditions on catalyst structure and composition will be examined very carefully. Methods for stabilizing particularly desirable combinations of structure and composition will be sought as part of this program.

Metal Carbides and Nitrides

As indicated in Table 1, a large number of the transition metals form stoichiometric carbides and nitrides. Considerable information is available concerning the structure and bonding of these materials, as a result of their importance to the metallurgical industries.[4,5] To a large extent, transition metal carbides and nitrides form interstitial compounds in which the carbon or nitrogen atoms are located in the voids between close-packed layers of the transition metal atoms. The presence of the interstitial atoms alters both the metal-metal bonding and the electron density at the metal atoms. Theoretical studies suggest that for carbides there is donation of electrons from non-metal to metal, while the opposite is the case for nitrides. Of considerable interest is the fact that the amount of charge transfer can be altered by changing the content of the non-metal.

The extent of prior research on the catalytic properties of transition metal carbides and nitrides has not been large.[2,6,7] Work done on Group IV to VI carbides has demonstrated that these materials can promote the isomerization, dehydrogenation, and hydrogenolysis of hydrocarbons. Of particular interest in this connection has been the observation that WC exhibits hydrogenolysis activity and selectivities resembling those of Pt and Pd, rather than W. The carbide and nitride of iron are both known to be effective catalysts for Fischer-Tropsch synthesis. Iron carbide produce primarily C_1-C_4 gas, C_5 liquids and wax. By contrast, iron nitride produces a relatively low molecular weight product with large yields of alcohols.

Intermetallic Compounds

Transition metals can form a very large number of intermetallic compounds.[2,3] Of principal interest for catalysis are silicides, borides (see Table 2) and intermetallics containing one of the rare-earth elements, RE. By contrast to carbides and nitrides, intermetallics containing B, Si, or RE do not form interstitial compounds, but instead exhibit crystal structures in which the metal-metal bonding is quite different from that of the transition metal alone. What makes these compounds potentially interesting catalysts is that their chemisorptive properties differ from those of the transition elements.

Research on the catalytic properties of intermetallic compounds containing transition metal elements is at a very early stage of development. Because of their higher stability, most of the work done so far has been with borides, particularly those of Ni and Co.[2] These materials have been found to be effective catalysts for hydrogenation, oligomerization, and methanation.[2,3]

TABLE 1

Standard Heats of Formation ($-\Delta H$ °)* of Select Nitrides and Carbides

Nitrides	TiN	80.4	VN	52	Cr_2N	27.3	Mn_4N	30.5	Fe_4N	3	Co_3N	−2	Ni_3N	0	Cu_3N	−18
Carbides	TiC	44.1	$VC_{0.88}$	24.5	Cr_3C_2	2.8	Mn_3C	4	Fe_3C	−5	Co_3C	−4	Ni_3C	−9	Unstable	
Nitrides	ZrN	87.3	NbN	57	Mo_2N	16.6	Tc		Unstable		Unstable		Unstable		Unstable	
Carbides	$ZrC_{0.9}$	47.0	NbC	33.6	MoC	~3			Low Stab.		Unstable		Unstable		Unstable	
Nitrides	HfN	88.2	TaN	59	Low stab.		Unstable		Unstable		Unstable		Unstable		Unstable	
Carbides	$HfC_{0.99}$	50.1	TaC	34.1	WC	9.7	Unstable		Unstable		Unstable		Unstable		Unstable	
Nitrides	LaN	71														

* ΔH_f in kcal/gm atom nonmetal)$^{-1}$ at 298 K.

TABLE 2

Standard Heats of Formation ($-\Delta H$ °)* of Borides, Silicides

Borides	TiB	38.3													
	TiB_2	22.3													
Silicides	TiSi	31	ViS_2	37	CrSi	19	MnSi	17	FeSi	19	CoSi	23	NiSi	20	
	$TiSi_2$	18			$CrSi_2$	15									
Borides	ZrB_2	38.0					Tc								
Silicides	ZrSi	37	$NbSi_2$	16	MoSi	14			$RuSi_{1.0}$	15.9	$RhSi_{1.0}$	16.1			
	$ZrSi_2$	19													
Borides	HfB	33.6													
	HfB_2	28.2													
Silicides			$TaSi_2$	12	WSi_2	11	ReSi	12	$OsSi_{1.0}$	15	$IrSi_{1.0}$	16	$PtSi_{1.0}$	15	

* ΔH_f in kcal/gm atom nonmetal)$^{-1}$ at 298 K.

Nickel silicides and nickel-intermetallics containing either La, Ce, Th, or Sm have been examined for synthesis gas conversion. All of these compounds are unstable under reaction conditions and decompose to form Ni supported on SiO_2 or ReO_x. It is significant to note though that the specific activity of the catalysts derived from the intermetallics compounds are significantly higher than those observed for conventionally prepared Ni/SiO_2.[3] Of additional interest in this connection are the results of recent work at Bell Laboratories, which has shown that the dehydrogenation and hydrogenolysis properties of Ni/SiO_2 and Ni/Al_2O_3 can be altered radically by thermal treatment with organic silanes, germanes, boranes, and alanes.[8] Characterization of the freshly prepared catalyst suggest that an intermetallic compound may have been formed near the surface of the supported Ni crystallites.

B. Proposal

The proposed program will be divided into three parts: catalyst preparation, characterization of bulk, and surface properties, and catalyst evaluation. Both bulk and supported catalysts will be used. It is anticipated that the use of an inert support such as SiO_2 or Al_2O_3 will be necessary to produce catalysts with sufficient surface area to be of interest for industrial application. Studies with bulk powders and single crystals will be conducted as well to obtain fundamental information regarding catalyst surface structure and composition. A certain number of comparative studies will also be conducted to help bridge the gap between work done with supported and unsupported materials.

During the first two years of the project, the focus will be on the carbides and nitrides of the Group IV through VI transition metals, and the silicides of the Group VIII metals. These materials will be examined in the form of single crystals, unsupported powders, and supported microcrystallites. Attention will be directed to establishing systematic variations in the structural, chemisorptive and catalytic properties of these materials as the composition of the transition metal is changed and as the stoichiometric ratio of metal to nonmetal is altered. Efforts will also be made to compare and contrast the properties of the catalysis studied with those of transition-metal catalyts. Particular emphasis will be placed on identifying the relationship between catalyst preparation and catalyst properties. For example, it will be of interest to determine whether compound catalysts can be prepared which affect hydrocarbon dehydrogenation, isomerization and dehydrocyclization with a minimum hydrogenolysis. Another focus for the initial work will be to explain why metal nitrides producing high levels of oxygenated products from CO and H_2 whereas metal carbides favor the synthesis of hydrocarbons. It is anticipated that information obtained from such investigations will help guide the synthesis of non-metal catalysts with desired properties.

Based on the initial results of the program, decisions will be made concerning the types of compounds to be investigated in later stages. This might include the study of mixed metal compounds or compounds containing two non-metal elements, such as carbonitrides, carbosilicides, etc. The exploration of rare earth-containing catalysts might also be pursued at that stage. The scope of adsorbates and reactants studied will be expanded during this phase of the project.

The technique used for catalyst preparation will depend on the type of material to be produced and its form. Thus, for example, where it is desired to work with single crystal or bulk powder metal carbides and nitrides, these materials will be formed by high temperature carbiding or nitriding of the metal. In this connection, it may be of interest to explore low-temperature plasma techniques for achieving non-stoichiometric compounds with unusual structures. Plasma-chemical methods might also be used to produce metal-compound catalysts directly from volatile metal-containing complexes. To achieve high surface area materials, it is proposed to deposit the active components on a support, such as silica or alumina. This might be achieved by first contacting the support with a volatile metal carbonyl and then

pyrolytically decarbonylating the complex to produce a high dispersion of the metal. The formation of a carbide, nitride or silicide could be accomplished by heating the dispersed metal in a gas such as methane, ammonia, or silane. In addition to the approaches noted here, attempts will be made to find novel synthetic routes for producing highly dispersed metal-compound catalysts.

Model, small surface area systems will be studied with the full repertoire of surface science techniques. This will include LEED for surface structure; AES, XPS, and ISS for surface composition; and UPS for characterization of the density of states in the valence band. The interactions of adsorbates with single crystals will be examined by means of EELS and TPD. The first of these techniques give information about the structure of the adsorbate and its interaction with the support, while the second provides information concerning the energetics of adsorbate surface. The ultra-high vacuum apparatus in which the model systems are to be examined will also be equipped with a low-volume isolation chamber. This chamber will be used for sample pretreatment at elevated temperatures and pressures, and for testing the catalytic performance of the sample. Results from these experiments will be of significant value for establishing links with the data obtained on powders.

The properties of supported catalysts, and catalysts in the form of unsupported powder, will also be examined using a variety of techniques. X-ray diffraction will be used, where possible, to establish bulk crystal structure. For both crystalline and amorphous samples, EXAFS will be used to determine meta-metal bond distances and average metal coordination numbers. Evidence for charge transfer between metal and nonmetal constituents will be sought using XANES, XPS, and UPS. Information on local bonding, coordination member, and the types of neighbors will be sought using solid-date NMR, with application of magic-angle spinning. Solid-state NMR will also be applied to gain insights into the nature of the local electronic structure of nonmetal elements (e.g., C, N, Si). Characterization of surface atoms will be attempted using recently developed echo and spin decoupling techniques [9,10]. If successful this would allow the geometry and electronic structure of surface atoms to be characterized and distinguished from those of bulk atoms.

The interaction of the catalysts with adsorbates will be examined using various spectroscopic techniques. Chief among these will be infrared spectroscopy. Since many of the catalysts are expected to transmit poorly in the infrared, observations will be made by means of diffuse-reflectance-infrared spectroscopy. The interactions of H_2, CO, and small hydrocarbon molecules with the catalyst surface will also be examined by means of solid-state NMR. Information from this technique will complement that obtained from IR spectra. The strength of adsorbate bonding will be characterized by TPD. This technique will also provide information regarding the extent to which adsorbate desorption is accompanied by decomposition. It is expected that these studies will provide important leads regarding the temperature range in which catalysis might occur and the initial steps involved in the progress of a catalyzed reaction.

Catalyst performance will be studied in microreactors designed to operate at pressures between 1 and 20 atm. Gas analysis will be carried out by gas chromatography. It is proposed that each catalyst be evaluated for several types of reactions. These might include cyclohexane isomerization, dehydrogenation, and hydrogenolysis; Fischer-Tropsch synthesis; and ammonia synthesis. CO oxidation and NO reduction should also be examined over these catalysts to determine their suitability for pollution abatement applications. Those catalysts which show unusually high activities and/or selectivity will be tested in an Xytel automated reactor system. This unit is designed for long-term performance studies and will provide data on catalyst stability..

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III. NOVEL MATERIALS IN CATALYSIS

A. Background

The synthesis of new catalytic materials such as novel inorganic and organic compounds of tailored structure, polymer immobilized catalysts, and homogeneous catalysts supported on solid particles constitutes a most important part of research in chemical catalysis.

This part of the document details an interdisciplinary effort in the exploration of novel approaches to potentially-catalytic materials of industrial interest. This will include the development of new heterogeneous catalysts with varied activity, surface reactions, reagent immobilization on electrodes for electrocatalysis, and the synthesis of novel monomers en route to organic and organometallic polymers.

The general aim of this work will be threefold:

1. to synthesize novel materials with potentially unique properties, activity and/or selectivity;
2. to characterize thoroughly these materials by spectroscopic and other means at the disposal of the organic, organometallic, polymer, solid-state, or theoretical chemist;
3. to evaluate their catalytic potential and other unusual properties such as conductivity, solid-state properties, stability, and so on.

Particular emphasis will be placed on the application of these materials to the catalysis of reactions of fundamental industrial importance in order to develop new systems and to understand the mechanism of their action. Examples will include hydrogenolyses of C-C, C-O, C-S, and C-N bonds, hydrocarbon isomerization, dehydrocyclization, oxidation, the Wacker process, reduction of CO and CO_2 with hydrogen to hydrocarbons, reduction of nitrogen, stereospecific reductions and oxidations of unsaturated organic compounds, and metal-mediated coupling and oligomerization reactions.

B. Proposal

1. Organic and Organometallic Chemistry on Surfaces

Much is now known about the mechanisms by which organometallic complexes mediate the interconversion of organic materials in homogeneous media.[1] One of the most intriguing recent developments in this area is the finding that electron-transfer reactions, of the type which often occurs at electrode surfaces, can greatly accelerate the rates of certain types of primary steps in homogeneous catalytic cycles. Specifically, it has been shown that the rates of ligand substitution reactions [eg (1)] and the reductive elimination reactions of alkanes from dialkyl metal complexes [eg (2)] can be accelerated by many orders of magnitude, when the number of electrons on the metal center is increased or decreased by oxidation or reduction processes.[2]

Many organotransition metal catalysts have been immobilized on solid supports, such as polystyrene[3] and silica[4]. Evidence in several cases is available that attachment to solid supports results in monodispersed materials. As a result, although the properties of these materials are not identical to those of their soluble relatives, their catalytic activity is often similar and observed differences are only quantitative (e.g., rates and selectivities can be modified).[5]

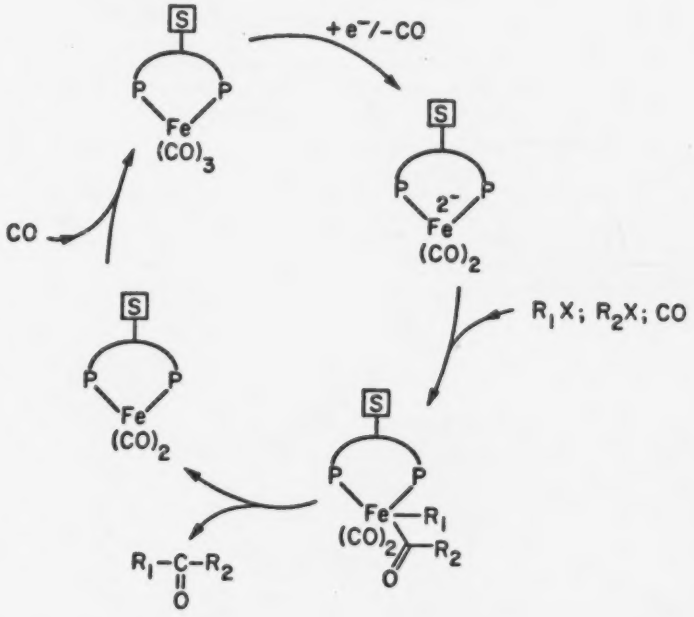
$$ML_n + L' \longrightarrow ML'L_{n-1} \quad (1)$$

$$L_nM\begin{matrix}R_1\\R_2\end{matrix} \longrightarrow L_nM + R_1\text{-}R_2 \quad (2)$$

We will utilize the techniques developed in the areas of supported catalysis, electron-transfer mediated catalysis, and deposition of organic materials on surfaces to generate supported organometallics to be exposed to one-electron redox reagents. Surface immobilization should impart stability to unusual oxidation states, which in turn should lead to the discovery of new reactions. A particularly intriguing possibility would be the utilization of electrocatalytic devices, such as surface-modified electrodes in order to control the oxidation states of the surface species under investigation. The proposed work will necessitate the preparation of novel organic and organometallic polymers with unusual conductivity behavior.

Below are outlined some specific examples of such systems. The first is based on a reduced iron species, known as "Collman's reagent" in homogeneous solution.[6] Its chemistry employs the Fe(O)/Fe(-II) couple to convert alkyl halides and CO into ketones. However, the lack of a method to resupply electrons to the extruded Fe(O) fragment, after reductive elimination of ketone, has prevented development of this reaction sequence as a catalytic process. We propose to immobilize ironcarbonyl onto a solid support [S]. As illustrated in Scheme 1, the supported metal center will

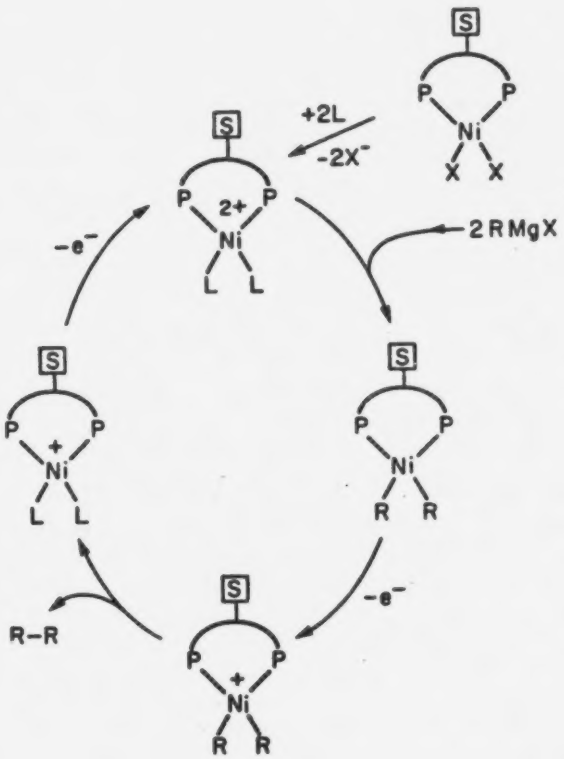
Scheme 1



then be reduced to the Fe(-II) state. Following alkylation, CO insertion, and reductive elimination of ketone, the supported Fe(O) product is re-reduced to Fe(-II), closing the cycle. The incorporation of Fe(O)/Fe(-II) centers on solid support particles should provide a method of electron transfer, and prevent aggregation of the Fe(O) product to unreactive cluster complexes. Such a sequence would provide a catalytic system for the double alkylation of carbon monoxide to give ketones.

A second example, illustrated in Scheme 2, utilizes an oxidizing electrode in a nickel-based system designed to couple organic Grignard or lithium reagents.[7]

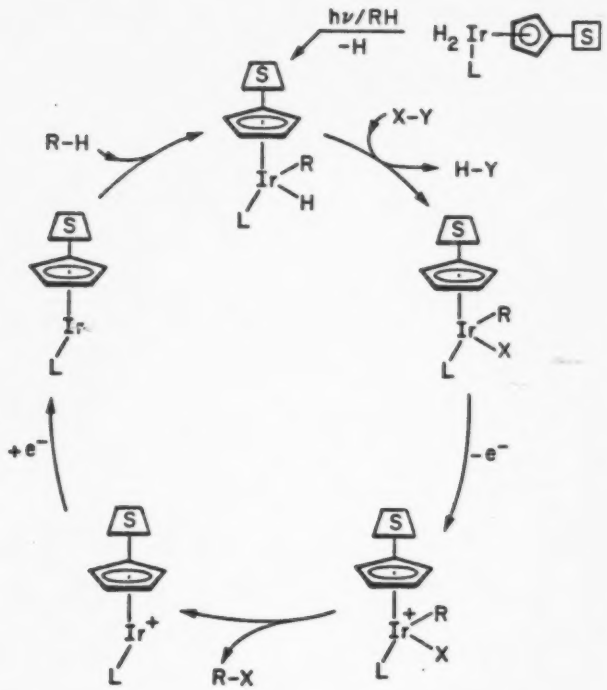
Scheme 2



Here nickel (II) halide is attached to the solid support. The halides are then displaced (possibly aided by electro-oxidation) by weakly-bound dative ligands (e.g., a coordinating solvent), represented as L. The metal center is doubly alkylated, and then oxidation is used to induce elimination. A second oxidation regenerates the initial (Ni(II) catalyst. In this way, a catalytic system for oxidative coupling of organometallic compounds might become available.

Finally, we illustrate in Scheme 3 a proposed method for functionalizing hydrocarbons using a recently-developed iridium C-H activation system.[8] Here the supporting electrode is used in both oxidative and reductive steps. The supported hydridoalkyliridium complex is generated by irradiating an appropriately substituted supported dihydride in the presence of an alkane. Known chemistry is used to replace the hydride ligand with a polar functional group X (e.g., hydroxide, halide, etc.).

Scheme 3



Subsequently electron transfer induced reductive elimination of RX takes place. This is followed by reduction of the supported iridium (II) fragment back to Ir(I), which is capable of closing the cycle by reacting with another molecule of hydrocarbon. Selective hydrocarbon functionalization in such a catalytic system would be immensely valuable as a new source of chemical feedstocks.

Should this chemistry prove successful, other catalytic and stoichiometric transformations involving redox cycles will be explored, as outlined in the background section.

2. Novel Polymers

Since the efficiency of the systems described in section 1 will benefit from the presence of supports capable of electron transport, novel polymers will be designed whose electronic

structure will facilitate such a process. In addition, these polymers will contain unusual capability in transition metal immobilization, and swelling properties commensurate with the requirements of the work outlined in sections 1 and 3. Thus, a combination of novel support-novel catalyst systems might lead to a new generation of potentially catalytic materials.

Some of these substances may be induced by doping to become conductors ("organic metals").[9] This field is very much in its infancy and promises to become one of the most exciting areas of polymer research. One of the obstacles to commercial utilization has been the lack of stability of the level of conductivity. There is also very little understanding of the relation between morphology, conductivity, and chemical reactivity.

In addition to their potential in catalysis, many other possible applications of conducting polymers have been proposed, the most immediate ones in certain areas of the aerospace and electronics industry. There is potential in the utilization of organic and organometallic conductors in low current circuitry, electromagnetic and electrostatic shielding, batteries, stabilized electrodes, semiconductor devices, and solar cells.

A common structural theme for these system is shown in Figure 1, the layering of organic and organometallic "sheets." The number of such layers might range from two to many. Layers may be ordered as shown, or disordered.

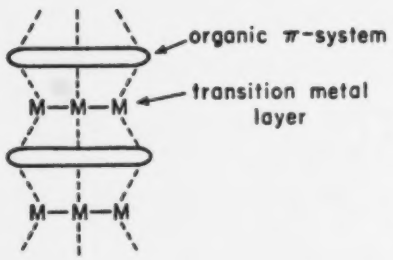
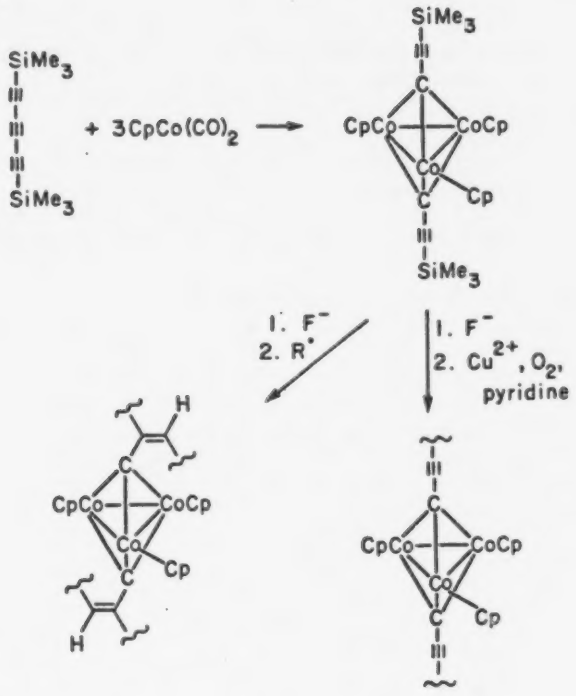


Figure 1 Novel multiple decker organometallic polymer

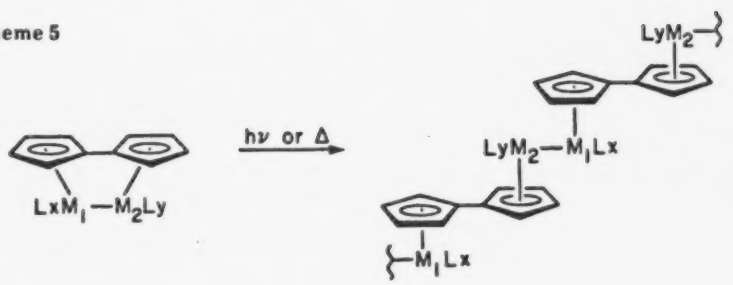
Potential approaches[10-12] en route to these systems are shown in Schemes 4-6. The potential of exchanging the metal in and out of the polymer by thermal, photo–, and other chemical means will be tested. Such exchange should provide access to a large variety of new systems with the incoming metal embedded in a predetermined polymer structure. Rigid optically active environments might give rise to enantioface-selective syntheses, particularly in catalytic hydrogenations of alkenes and of carbonyl compounds, and in carbon-carbon bond forming reactions.

G-20

Scheme 4



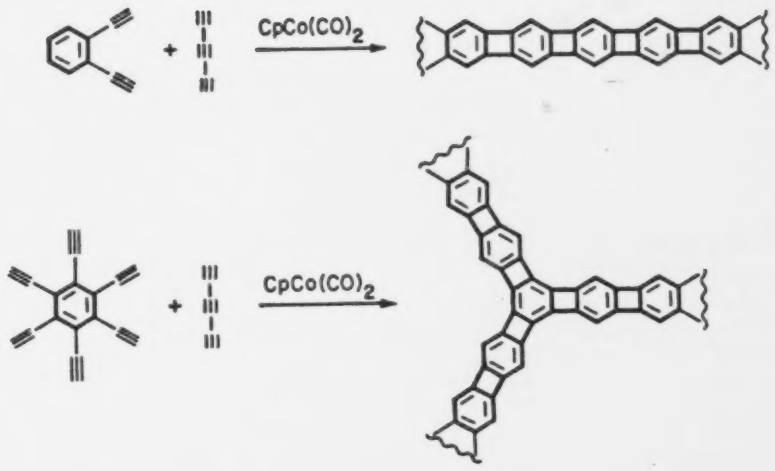
Scheme 5



M = metal
L = ligand

G-21

Scheme 6



It might also be possible to effect shape-selective reactions by copolymerization of monomers in the presence of zeolites, and the subsequent attachment of additional immobilized catalysts to the polymer backbone. An example would be the reduction of carbon monoxide to give methanol trapped in a (polar?) polymer matrix to be released as a hydrocarbon of specific size after interaction with the zeolite. Another example would involve a catalytic dehydrocyclization-rearrangement sequence leading to specifically substituted aromatics.

3. Novel Electrodes in Electrocatalysis

In section 1, novel approaches to the generation of potential catalysts in unusual oxidation states were described. One such approach might rely on electrocatalytic techniques. In order to embark on this course of research it is necessary to design functional molecular assemblies at electrodes which would allow, on the one hand, confinement of a catalyst within a thin film at the electrode surface and, on the other hand, would provide appropriate means of electron and ion transport across such assemblies.

Over the past years several methods have been developed for the attachment of monolayers of various reagents at electrode surfaces.[13,14] They rely on the irreversible adsorption or chemisorption, or on the covalent attachment of reagent molecules to surface functional groups (e.g., carboxy groups on graphite electrodes, hydroxy groups on metal oxides). Collman, et al. adsorbed a cofacially sandwiched cobalt porphyrin complex on a graphite electrode and observed catalyzed electroreduction of dioxygen to water.[15,16] Unfortunately, the system suffers from instability of the modified electrode surface due to the desorption and/or decomposition of the catalyst. More stable chemically-derivatized surfaces are obtained when an electrocatalytically-active reagent is immobilized in a thin film of a polymeric matrix coated on the electrode surface.[17-20]

Various methods have been proposed to study electron transport process across polymer films at electrodes.[33-35] A major difficulty associated with the polymer-modified

electrodes has been the intrinsically small values of the effective diffusion coefficients, D_{eff}, which describe the overall rate of electron transport. Values for D_{eff} as low as 10^{-10} - 10^{-12} cm^2/s are not uncommon and are due to the insufficient swelling of the polymeric film.[30,36-40]

Studies will be initiated and aimed at the preparation of thin polymer films with variable swelling characteristics at electrodes which would allow faster electron transport. In this work some of the novel polymers developed in section 2 will be tested.

Polymer films stable in water (or polar solvents) will be prepared by spin-coating soluble polymers on electrode surfaces followed by chemical cross-linking to a degree which will allow the appropriate extent of swelling in aqueous (or organic) solutions. Ion-containing polymers will be of primary interest as they can electrostatically bind ionic electroactive species.

In another approach radical polymerization of vinyl monomers will be used to create *in situ* a cross-linked polymer film on the electrode surface. These surface polymerized matrices can then be used to entrap other types of polymers or large monomers that are electroactive or serve to immobilize desired electroactive species. The characterization of these polymeric matrices will involve measurements of the extent of their swelling and permeability to ion migration. The electrochemical behavior of the electroactive reagents incorporated into a polymeric film and stability of these films will be studied. Electrochemical measurements of the effective diffusion coefficients of electron transport will determine the usefulness of these films as electron mediator layers.

There have only been sporadic reports of catalytic applications of electrodes with polymer electrocatalytic films. Miller et al. demonstrated catalyzed electro-oxidation of NADH by polymer-bound dopamine.[13] The same group also effected the catalyzed reduction of 1,2-dibromo-1,2-diphenylethane to stilbene at a Pt electrode coated with poly(p-nitrostyrene).[42] Anson et al. have recently reported on the electro-reduction of dioxygen to water catalyzed by a Ru(III)-histamyl complex covalently attached to an acrylate copolymer film at a graphite electrode.[43] In other reports the electrocatalytic oxidation of oxalate[44] and ascorbic acid[45] have been communicated.

In our approach we will develop surface-bound electrocatalytic assemblies which would be heterogeneous in their chemical structure. A schematic model of such an assembly is shown in Figure 2.

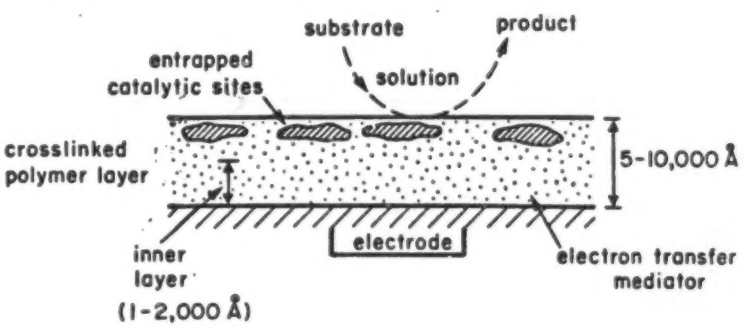


Figure 2 Simple picture of electrocatalysis with polymer embedded catalysts on electrode surfaces. The catalysts may be transition metals, zeolites, and organic materials.

The electrode film is essentially composed of two functionally different parts. The outermost layer of assembly contains an electrocatalyst. The catalyzed redox conversion of reagents to products will take place within this layer. The inner layer links the catalytic layer with the electrode; it will contain an electron transfer mediator. Its role is to continously regenerate the catalyst by transporting electrons between the catalyst and the electrode.

The various catalytic materials which will be synthesized can be classified as either solid particle type (zeolites, catalysts supported on inert oxides) or macromolecules (polymer-bound catalyst, etc.).

Solid particles (with a diameter in the submicron range) will be entrapped in a layer of, for example, crosslinked acrylamide-gel, polymerized *in situ*. Since these particles will be large and will contain catalytic sites confined to their surface, one will have to ensure that the mediator reaches deeply into the catalytic layer (Figure 2). To achieve this the layer of acrylamide-gel with the entrapped particles will also have to contain the mediator binding polymer. The incorporated mediator will then have good contact with the catalyst sites.

The same concern is valid in the case where a catalyst is a macromolecular species. The catalyst layer (an outer film) and the mediator layer must both be swellable in the solvent used in the electrochemical experiments. Otherwise only a very thin film of catalyst may overcoat the mediator layer without blocking the electron transport chain. The choice of the mediator will depend on a particular type of the catalyst used.

After the preparation and characterization of such novel electrodes, model electrocatalytic systems will be designed in order to test the potential of the approach as described in section 1. If successful, industrial applications may readily be envisaged, since the electrode efficiency should ideally be only mass-transport and surface-dependent, as seen in classical electrolysis.

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IV. PERSONNEL

This project will require participation of an interdisciplinary group of scientists, involving LBL staff, University of California, Berkeley faculty, graduate students, and visiting industrial and university associates. It will also serve as a training opportunity for future scientists.

While a number of new scientists are expected to be hired (e.g., a colloid chemist), identified participants thus far are:

Andersen, R., UCB (*inorganic synthesis*)

Bell, A.T., UCB/LBL (*chem. eng.*)

Bergman, R.G., UCB/LBL (*organic chemistry*)

Gronsky, R., LBL (*electron microscopy*)

Heinemann, H., LBL/UCB (*process technology and catalysis*)

Maier, W., UCB (*organic chem.*)

Majda, M., UCB (*electrochemistry*)

Michaels, J.W., UCB (*chem. eng. - spectroscopy*)

Pines, A., UCB/LBL (*NMR*)

Radke, C.J., UCB/LBL (*colloid chemistry and engineering*)

Reimer, J., UCB (*NMR*)

Somorjai, G.A. UCB/LBL (*physical chemistry*)

Stacey, A., UCB (*inorganic synthesis*)

Templeton, D.H., UCB/LBL (*x-ray spectroscopy*)

Vollhardt, K.P., UCB/LBL (*organo-metallic catalysis*)

The actual research will be conducted by graduate students and postdoctoral students working with the principal investigators. Once the program has been established, efforts will be made to hire one or more highly qualified scientists into LBL. Such individuals would have responsibility for a portion of the scientific program.

The participation of industrial researchers will be sought from the onset of the program. It is expected that such individuals would come to NCAM for six months to a year, to study the properties of particular catalysts being investigated by the principal investigators, or to characterize materials developed in their company, using techniques available at NCAM.

V. INTERACTIONS WITH INDUSTRY

An important aspect of the program will be to promote the exchange of people and information with industry. The exchange of information will be accomplished through seminars and symposia on advances in metal-compound catalysts, held periodically at NCAM. The NCAM investigators will also be available to give seminars on specific topics at industrial laboratories. The ultimate goal of these efforts will be to keep industrial researchers apprised of the studies ongoing at NCAM and to seek advice and input into the NCAM program. It is hoped that such interactions will assist in the development of novel catalyst materials that are of significant interest to American industry.

Several industrial organizations in the petroleum, petrochemical, chemical and catalyst manufacturing industries have expressed interest in potential collaboration in this program. Discussions have been held with two outstanding and world-renowned industrial specialists in zeolite synthesis and characterization, who have indicated their willingness to spend six months to a year at LBL to assist the project in its initial phases and to provide background experience. A commitment on their part is, of course, subject to their company's management approval, which cannot be sought until the project has been approved and funded.

Similar discussions have been and are being held with industrial scientists to participate in the other parts of this program. There has been a very positive reaction always, subject to company approval. In addition, several companies have expressed their desire to send people for a few days for discussion of parts of the program that are of particular interest to them and for exchange of information. This, of course, is only feasible once the program is staffed and underway.

DOE/S-0027

Materials Research and Development

Prepared by the Materials Research and Development Panel

November 1983

A Report of the
Energy Research Advisory Board
to the
United States Department of Energy
Washington, D.C. 20585

Energy Research Advisory Board
to the
United States Department of Energy
1000 Independence Avenue, S.W.
Washington D.C. 20585
(202) 252-8933

November 30, 1983

Honorable Donald Paul Hodel
Secretary of Energy
Washington, D.C. 20585

Dear Mr. Secretary:

I am pleased to forward the Energy Research Advisory Board's (ERAB) Report on Materials Research and Development prepared by the Materials R&D Panel. This report, unanimously approved by ERAB on November 4, 1983, was prepared in response to the Deputy Secretary's request of November 2, 1982, to undertake a review that would help the Department ensure that our materials R&D programs are pursuing appropriate research goals and effective interfaces exist with other agencies and the private sector.

While the principal points are summarized in the Report's Executive Summary and the Panel Chairman's letter, there is one additional issue we wish to highlight. Namely, as budgetary pressures increase it becomes increasingly difficult for new investigators to enter the field. The Report does not make any specific recommendations regarding this matter, but the Board is aware of the Department's recognition of this as a problem not only for materials scientists but for all scientists in both the national laboratories and in the universities.

I trust that these findings and recommendations will be of use to the Department in formulating materials R&D policy.

Sincerely,

Louis H. Roddis, Jr.
Chairman
Energy Research Advisory Board

Enclosure

October 21, 1983

Mr. Louis H. Roddis, Jr.
46A State Street
P. O. Box 1513
Charleston, SC 29402

Dear Lou,

I am pleased to submit the final report of the Panel on Materials Research and Development to the Energy Research Advisory Board for consideration at its meeting on November 3-4, 1983. The final report completes the Panel's work in connection with the Deputy Secretary of Energy's request for ERAB to review DOE's materials programs to assist the Department in ensuring that the programs are pursuing appropriate research goals and that effective interfaces exist with other agencies and the private sector.

The principal findings of the Panel relate to (1) the need for a stronger focus within the energy technology offices and the delegation of broader responsibilities to the nondefense energy laboratories, and (2) the need for a technology development program to bridge the gap between materials research funded by Basic Energy Sciences and materials engineering funded by the applied technology divisions. There is general agreement among Panel members on the findings and recommendations.

The Panel very much appreciates the cooperation of the laboratories, operations offices, and Headquarters in this effort. To facilitate ERAB's review, I am sending the report to all Board members by copy of this letter.

Sincerely,

Robert H. Ray
Chairman, ERAB Materials R&D Panel

RHP/a
attachment

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CONTENTS

I. EXECUTIVE SUMMARY 1

II. MOTIVATION AND CHARGE 5

III. BACKGROUND 7

A. History 7

B. Organization 7

IV. CONDUCT OF THE STUDY 11

V. FINDINGS AND RECOMMENDATIONS 15

A. What are the basic materials research roles of DOE and what is the proper balance among roles and among performers? . . 15

B. What portion of the DOE basic materials science budget should be allocated to the development and support of major facilities? 16

C. Are the responsibilities assigned to the nondefense laboratories adequate to allow the effective development of relevant materials programs? 18

D. Are there important gaps in the materials programs? 21

E. How can the results of materials R&D programs be more effectively incorporated into energy developments? 22

VI. REFERENCES AND BIBLIOGRAPHY 25

APPENDIX A, DEPUTY SECRETARY'S CHARGE A-1

APPENDIX B, PANEL MEETINGS AND SITE VISITS B-1

I. EXECUTIVE SUMMARY

The performance of materials is central to the economic, reliable and efficient production and utilization of energy and the development of new energy and defense technology. Recognizing this, the Department of Energy (DOE) and its predecessor agencies, the Atomic Energy Commission and the Energy Research and Development Administration (AEC and ERDA), have always maintained strong materials research and development (R&D) programs. DOE is currently the largest single source of documented materials research and development funding in the United States — in excess of $300 million per year. In view of the importance and extent of materials research and development within DOE, the Energy Research Advisory Board (ERAB) was asked "to undertake a review that would help the Department ensure that . . . [its] programs are pursuing appropriate research goals and that effective interfaces exist with other agencies and the private sector." The Board established the Materials R&D Panel to carry out this review.

The review has concentrated on the question of how DOE organizes and conducts its materials R&D programs rather than evaluating specific programs. Input was solicited from DOE program managers, visits made to many DOE energy and defense laboratories, and subpanels were established to look into R&D relationships with universities and industry. The following are the key questions posed to the Board in its charge (Appendix A).

- Are DOE energy and defense systems materials needs effectively translated into materials research programs and directed toward solving these specific problems, and are the results of these materials programs adequately incorporated into energy developments?

- Are there important new opportunities in materials research that have been overlooked or are not being adequately addressed by DOE materials programs or elsewhere?

- Is the coordination of materials research programs between Government, national laboratories, universities, and industry effective with respect to resource allocation and utilization of results?

- What is the significance and role of the DOE materials science programs relative to the Nation's overall effort in materials R&D, especially with the development and support of major materials research facilities; how can the national contribution and benefits from DOE materials science programs be further enhanced?

These four key questions raise several basic underlying issues. How these issues relate to the charge questions is mapped on page 13 of the report. The five critical issues and the Board's findings and recommendations relative to each follow.

A. What are the basic materials research roles of DOE and what is the proper balance among roles and among performers? The Board concluded that the Department has three basic materials research roles relative to the nation's overall effort in materials: (1) to provide basic knowledge necessary for the long-term support of DOE energy and defense missions; (2) to support university research necessary for the education of graduate students who will most likely contribute to national energy and defense objectives; and (3) to operate unique large facilities that support basic materials research and make these facilities available to university, industry, and government researchers in materials science. To ensure a planned and measurable balance between these purposes, the Basic Energy Sciences (BES) should explicitly provide appropriate core funding for the basic materials research required to make the use of unique large facilities most effective. All other BES materials programs should be competitively funded in DOE laboratories and universities within the guidelines of providing high-quality science results with long-range relevance to DOE energy needs, coupling basic materials research to technology development, and training future scientists and engineers.

B. What portion of the DOE basic materials science budget should be allocated to the development and support of major facilities? In the past decade there has been a significant increase in the fraction of the BES materials budget allocated to the construction and operation of large facilities (about 10% to 20%). When budgeting for additional facilities, DOE management should ensure that the cost of operating and maintaining such facilities does not adversely affect the rest of the materials science program.

C. Are the responsibilities assigned to the nondefense laboratories adequate to allow the effective development of relevant materials programs? The responsibilities of the energy laboratories need to be redefined and sharpened to improve their conduct of materials R&D. The assignment of responsibility should have the stability necessary for attacking and solving major long-range problems. The Assistant Secretaries for Nuclear, Fossil, and Conservation and Renewable Energy should develop a stronger focus within their offices and delegate broader responsibilities to the nondefense energy laboratories than is now done under current DOE policy on lead laboratories. These assignments should focus on some energy system or technology such as coal conversion or breeder reactors or a subsystem such as pressurized gasifiers or breeder fuel or containment and should include overall system or subsystem responsibilities. The lack of well-defined responsibilities has resulted in the lack of well-defined research priorities and thus in a nonoptimal allocation of resources. As better-defined responsibilities are delegated to the laboratories, DOE program managers should concentrate on defining areas of energy system relevance and need and on maintaining budget accountability, leaving the detailed management of materials programs to the laboratory management. Independent supporting R&D funds should be provided to the laboratory directors to perform the basic and applied research required to underpin the assigned energy missions, and the laboratory directors should then be held accountable for the successful accomplishment of the missions.

For some energy laboratories, development and management of unique large facilities such as intense neutron and X-ray sources, along with the concomitant research necessary to maintain expertise, should constitute their principal mission.

D. Are there important gaps in the DOE materials programs? The Board finds that there is a gap between materials research and materials engineering in DOE materials programs and recommends establishing under each Assistant Secretary a needs-oriented technology development program along with an identifiable budget category. Such technology development programs should be funded in parallel with systems development programs, not under them, and should be assured of the continuity of funding required to complete the development of materials to the point of readiness for system application.

E. How can the results of materials R&D programs be more effectively incorporated into energy developments? The Board recommends that DOE provide clearly defined incentives, such as exclusive licenses, for industry to show greater initiative in technology transfer. DOE should seed materials research programs at selected universities, which also have state and/or industrial support, to promote technology transfer to industry and proliferation of entrepreneurial companies. Management of national laboratories should be evaluated in part on their success in promoting innovation and technology transfer. DOE should also be more active in identifying and transferring to the U.S. energy-related materials research results obtained in foreign laboratories.

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II. MOTIVATION AND CHARGE

In the past, major advances in DOE energy and defense systems have depended in large measure on development of new and improved materials. Consequently, the DOE and its predecessor agencies, AEC and ERDA, have maintained substantial materials R&D programs. In fact, DOE, which supports more than one-third of all recognized federally funded materials R&D,* is currently the largest single source of documented materials R&D funding in the federal government. DOE programs range from basic research in solid state physics and chemistry to materials and process engineering development for specific energy and weapons systems. The Department is prominent among government and private sources of funding for materials R&D in universities and in support of major facilities for materials research and analysis.

Recognizing the importance of materials R&D to the mission of DOE and the need to strive continually for its improvement, the Deputy Secretary requested that ERAB undertake a study of the Department's materials R&D (Appendix A). The Board was asked to "undertake a review that would help the Department ensure that interfaces exist with other agencies and the private sector."

The Deputy Secretary hoped "in particular, . . . that the ERAB study could consider these key questions":

- Are DOE energy and defense systems materials needs effectively translated into materials research programs and directed toward solving these specific problems and are the results of these materials programs adequately incorporated into energy developments?

- Are there important new opportunities in materials research that have been overlooked or are not being adequately addressed by DOE materials programs or elsewhere?

- Is the coordination and coupling of materials research programs between Government, national laboratories, universities, and industry effective with respect to resource allocation and utilization of results?

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*In this and subsequent sections, research and development (R&D) refers to definitions of the phases of R&D set forth in the Schedule and Format Instructions for Multiprogram Laboratory Institutional Planning dated April 1982. For this study, the Board has used the aggregated categories of research, technology development, and engineering (defined on p. 11c.

- What is the significance and role of the DOE materials science programs relative to the Nation's overall effort in materials R&D, especially with respect to the development and support of major materials research facilities; how can the national contribution and benefits from DOE materials science programs be further enhanced?

Subsequent to the receipt of the Deputy Secretary's charge, the Materials R&D Panel was assembled (list of members follows transmittal letters). It began investigation in January 1983 and undertook to answer these four questions as its basic mission.

III. BACKGROUND

A. History

There has been a strong emphasis on materials R&D throughout the existence of DOE and its predecessor organizations. The materials R&D in AEC supported the nuclear mission of that agency in reactors and weapons. With the formation of ERDA in 1975, materials R&D was broadened to include support for all energy technologies. Materials programs were developed in the fossil, conservation, and solar areas; and Basic Energy Sciences (BES) materials research shifted toward nonnuclear technologies. Data on DOE materials R&D funding in the past ten years (Table 1) indicate some expansion in DOE materials R&D funding (particularly in BES) over the past five years, but significant reductions in materials R&D in the nonnuclear technologies paralleling reductions in the overall DOE effort in these areas.*

B. Organization

Materials R&D programs are dispersed throughout the research and technology offices of DOE (see Table 1, p. 8). Basic materials research and magnetic fusion materials R&D are performed within the Offices of BES and Fusion Energy (FE), respectively, which are under the Office of Energy Research. Materials R&D for the other energy technologies is performed within those technology offices. Communication among the various materials programs is through the Energy Materials Coordinating Commmittee (EMaCC) (Ref. 4) and through informal contacts and workshops. EMaCC includes materials representation from BES and each of the energy technologies and meets periodically to exchange information. The interagency Committee on Materials (COMAT) serves a similar function for the various materials programs in the federal government. Within DOE there is no single office or advisory committee with a policy responsibility for the materials R&D program.

DOE has become custodian of most of the federal Government's major materials research facilities. This situation reflects DOE's substantial support for basic materials research and the unique attributes of the national laboratories for operating large facilities. The DOE materials research facilities budget is more than double that of the National Science Foundation (NSF). The emphasis on facilities-related research has increased significantly in the past decade, and facilities operations now account for nearly 20% of the DOE Materials Sciences Division budget. These facilities are becoming increasingly accessible to outside users and have a substantial impact on research choices in the materials community.

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*Additional background information can be found in the appendices and in Refs. 1–4.

Table 1. DOE materials R&D budgets for FY 1973 through FY 1983[a]

	Operating Funds (millions of dollars)										
	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983
Conservation and Renewable Energy											
Solar[b]				12	20	28	32	34	32	28	27
Conservation	NA[c]	NA	NA	NA	NA	19	28	30	26	22	22
Defense Programs[d]	53	63	62	58	65	84	74	71	78	98	104
Energy Research											
Fusion			5	6	9	8	9	10	12	15	17
BES[e]	24	32	40	44	53	60	68	78	87	96	108
Fossil Energy	NA	NA	NA	NA	NA	30	32	24	28	20	18
Nuclear Energy[f]	NA	NA	NA	NA	NA	69	75	113	78	81	69
Resource Applications[g]						7	13	14			
Totals						305	331	374	341	360	365

[a] Reported by the Energy Materials Coordinating Committee and modified by Panel staff to provide consistent basis.

[b] Primarily in the National Science Foundation prior to 1976.

[c] Data not available.

[d] Includes classified and nonclassified defense materials research and development (R&D), inertial confinement fusion materials R&D (beginning in 1978), and defense wastes R&D (beginning in 1982).

[e] Basic Energy Sciences.

[f] Includes materials R&D for breeder reactors, naval reactors, other fission reactors, and civilian wastes.

[g] Phased out in 1981.

The DOE role in the operation of materials research facilities is often considered a national trust activity and is not justified solely on its relevance to energy materials research.

DOE is a substantial source of materials research funds for universities (nearly half the NSF total in 1982). Accordingly, DOE significantly influences the overall strength and directions of materials research and the research specialities of graduate students. The major materials research facilities are also utilized by faculty and students.

DOE materials R&D programs are performed by the multiprogram national laboratories,* universities, and industry. The DOE national laboratories represent a significant national resource for research and development. Each laboratory is unique and often serves in a variety of different roles. The weapons laboratories have a clear mission in defense programs; Oak Ridge and Argonne are major energy technology R&D centers; and the Brookhaven, Ames, and Lawrence Berkeley laboratories emphasize different aspects of basic energy science. In addition, some laboratories are assigned a contract management or "lead laboratory" role for certain DOE programs. In the materials area, national laboratories perform basic and applied research, engage in engineering development, and operate national facilities.

DOE materials R&D programs in universities vary from individual contracts to large materials research laboratories such as Illinois, Ames, and Lawrence Berkeley. (The latter two are national laboratories located on university campuses.) The university programs primarily perform generic basic materials research and provide the nation with scientific manpower. Industry plays a smaller role in DOE materials R&D programs. This is a consequence of the long-range nature of the DOE research effort in the energy technologies. Most of the current industry involvement is in the fission, fossil, and conservation programs.

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*The multiprogram laboratories (as covered in Ref. 6) are Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Berkeley Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest Laboratory, and Sandia Laboratories.

IV. CONDUCT OF THE STUDY

In carrying out this study, the Board was guided by the four key questions posed in its charge letter. Early in its deliberations the Board recognized that it was thereby confronted by two principal tasks. The first was to examine in some depth how DOE organizes and conducts its materials science and technology base programs. The second was to examine how well DOE manages these programs.

It appeared that complete answers to the four key questions would depend upon carrying out both these tasks. However, in view of the limited time and resources available, it was not considered feasible to carry out in depth the examination of the quality and impact of substantive materials research programs implied by the second task. Moreover, the Board considered it far more important to concentrate on determining whether DOE had in place the necessary organizations, assignment of responsibilities, and motivations to enable the conduct of an excellent materials science and technology program.

To provide a common basis for this report, the various categories of research, technology development, and engineering needed to be defined. DOE has used a variety of definitions in the past, but the following definitions were used in this study: Research includes basic and applied research, from fundamental research to systematic studies directed toward developing a fuller scientific knowledge needed to fulfill specific requirements. Technology development covers both exploratory and advanced developments that ultimately lead to a demonstrated proof of principle for a particular application or product. Engineering refers to the systematic use of materials to achieve a detailed design, to support the testing and evaluation of system prototypes, or to validate the performance and reliability of pilot plants.

Emphasis placed by the Board on the organization and conduct of programs stems from an important distinction between the materials research and technology development programs and the engineering programs in respect to the way in which systems needs are expressed and met. Materials engineering programs are aimed to meet short-term systems needs that can be expressed in terms of specific problems needing immediate solution. Materials research and technology development programs are designed to take a longer-term approach and generally have their major impact on energy or defense systems needs five to ten years after inception. On this time scale, materials needs are necessarily expressed in broader and more generic terms, and the relevance and success of programs depend heavily on how well the programs are motivated, organized, and conducted.

Some of the key factors involved are the following: explicit mechanisms for translating systems needs into relevant programs, the coupling of research and technology development programs to engineering

programs, the existence of management methods for monitoring the quality of research and technology development programs by scientific and engineering community standards, the aggressive application of new science and technology to systems needs, and in the case of established laboratories a well-defined mission. Industrial experience has provided abundant evidence of the importance of these factors.

Effectiveness in dealing with these factors, the Board feels, gives the best assurance that DOE energy and defense materials needs will be translated into effective and relevant research programs, productively coupled to system needs. It was therefore decided to concentrate on the effectiveness with which the necessary functions in the chain of research, technology development, and engineering are performed and are coupled together. This decision was strengthened by early indications and advice to the Board that no explicit methods exist in DOE for closing the loop between system needs on the one hand and research and technology development on the other and that exploratory programs in materials science do not usually result in effective transfer of technology to systems outside the defense programs.

After analyzing the four key questions in its charge letter, the Board recognized that to reply in a factual and useful way, several basic underlying issues would have to be separately identified and addressed. The five most critical underlying issues reflect the strongly held view of the Board that its most important task was to understand how DOE organizes and conducts its materials R&D programs. These critical issues are formulated in the following questions.

A. What are the basic materials research roles of DOE and what is the proper balance among roles and among performers?

B. What portion of the DOE basic materials science budget should be allocated to the development and support of major facilities?

C. Are the responsibilities assigned to the nondefense laboratories adequate to allow the effective development of relevant materials R&D programs?

D. Are there important gaps in the DOE materials programs?

E. How can the results of materials R&D programs be more effectively incorporated into energy developments?

Answers to the four key questions posed to the Board in its charge letter depend upon the findings concerning these five critical issues. The key questions are related to the critical issues as follows:

Key questions	Critical issues
Are DOE energy and defense systems materials needs effectively translated into materials research programs and directed toward solving these specific problems, and are the results of these materials programs adequately incorporated into energy developments?	C, D, E
Are there important new opportunities in materials research that have been overlooked or are not being adequately addressed by DOE materials programs or elsewhere?	A, C
Is the coordination and coupling of materials research programs between Government, national laboratories, universities, and industry effective with respect to resource allocation and utilization of results?	B, C, E
What is the significance and role of DOE materials science programs relative to the Nation's overall effort in materials R&D, especially with respect to the development and support of major materials research facilities; how can the national contribution and benefits from DOE materials science programs be further enhanced?	A, B, C, E

The Board did not attempt to review in detail the technical merits of each DOE materials program. Recent studies provide ample evidence that DOE basic materials research is of high scientific quality (Ref. 1). In this study the Board has concentrated on how DOE chooses and conducts its materials programs. In particular, the study addressed issues of planning, decision making, interfaces, and balance in DOE programs. The study attempted to determine whether DOE is pursuing appropriate materials goals, with effective interfacing and attention to transfer to industry for commercialization and with an appropriate balance of effort.

In carrying out its study, the Board relied on input from DOE program managers, national laboratories, universities, and industry. Subpanels were established to look into DOE materials R&D relationships with universities and industry. Site visits were made to most of the DOE multiprogram and weapons laboratories (see Appendix B for a list of Panel meetings and site visits), and a detailed survey of DOE-operated national materials research facilities was conducted.

The intent of the study was to include an examination of all DOE work in materials. Full cooperation was received from the Department of Defense (DOD) and other government agency materials programs and from most DOE programs. The single exception was the DOE Naval Reactor Program, whose managers declined to participate in this study. Consequently, no reference is made in this report on the conduct of its programs, its effectiveness, or its ability to interact with other groups.

V. FINDINGS AND RECOMMENDATIONS

A. What are the basic materials research roles of DOE, and what is the proper balance among roles and among performers?

Findings:

The DOE BES Program provides a significant fraction of the funding for basic materials research in the United States. This BES materials research is carried out in the DOE multiprogram laboratories and university laboratories, with a minor amount of research carried out in other institutions. A significant fraction of these research funds (about 20% in 1983) is spent for the operation and maintenance of unique large facilities (described in Section B) situated primarily at the DOE multiprogram laboratories.

The mission-oriented energy and defense programs conducted at DOE multiprogram laboratories require a basic research program in related materials areas to develop new materials, principles for solving problems with commercially available materials, and materials processing procedures and to provide both a window to external world science and a means for coupling scientific expertise to the applied programs.

These needs for basic materials science work within the multiprogram laboratories must be balanced with both DOE and U.S. needs to maintain a strong basic materials science competence in U.S. universities. Universities must continue to provide both outstanding research in basic materials science and a steady flow of advanced-degree scientists and engineers able to carry out the research and technology efforts in support of broad DOE and national needs.

Because DOE multiprogram laboratories are the managers of most of the unique large facilities, they must maintain a certain level of in-house basic research expertise associated with each facility. This core effort is needed to provide laboratory management with expert advice on machine performance and upgrades and to provide an expert group to advise on research carried out and techniques used in these facilities by others.

The Board concludes that DOE has three basic materials research roles relative to the nation's overall effort in materials. These are (1) to provide basic knowledge necessary for the long-term support of DOE energy and defense missions; (2) to support university research necessary for the education of graduate students who will most likely contribute to national energy and defense objectives; and (3) to operate unique large facilities that support basic materials research and make those facilities available to university, industry, and government researchers in materials science.

The Board found that these three roles of the DOE basic materials program are often not sufficiently delineated when justifying programs in the multiprogram laboratories or university laboratories. As a consequence, it is difficult to determine the balance among the roles or to plan what the balance should be when other national programs are taken into account.

It is important that DOE maintain a recognizable and measurable balance among the three basic materials research roles. Lack of such measurable distinction leads to confusion with respect to the needed size and specific direction in each role. Specific means should be sought to provide this balance through an improved allocation of funds. The following recommendations address this issue.

Recommendations:

Funds for the routine technicians support are normally provided for in operating budgets for unique large facilities. In addition, BES should also explicitly provide appropriate core funding for basic materials research performed in those facilities by the host laboratory. Such professional technical funds should be allocated to laboratory management to ensure needed expertise surrounding these facilities. The amount of such funding should be decided by the DOE program office on a case-by-case basis depending upon the need for such expert facility support and technical direction.

All other basic materials science research funds should be granted by BES on an open competitive basis between university, multiprogram, and other laboratories. The decision bases for competitively granting such funds should be (1) the quality of the research and long-term relevance to the DOE energy mission, (2) the need for coupling basic materials research to technology development, and (3) the graduate education value of the research.

B. What portion of the DOE basic materials science budget should be allocated to the development and support of major facilities?

Findings:

In the past decade there has been a significant increase in the fraction of the BES budget allocated to the construction and operation of large research facilities. Facilities operations now account for nearly 20% of the DOE Materials Science Division budget (Table 2, p. 17).

It is not unreasonable for BES to have a large part of its budget allocated to such facilities, since DOE has become custodian of most of the nation's major materials research facilities. In part the increase represents new facilities built under DOE Materials Science sponsorship in response to perceived needs for materials research. (In some instances, the Materials Science Program has been given the responsibility of building and operating facilities to serve needs much broader than materials research.) In part the increase represents facilities built by other agencies but transferred to DOE to operate.

Table 2. Materials Science Division (BES) expenditures for major facilities operation

Fiscal year	Facility operation budget (millions of dollars)	Total division budget (millions of dollars)	Percent
1970	3.1	27.9	11.1
1974	3.4	32.1	10.6
1981	12.3	87.5	14.1
1982	15.1	95.5	15.8
1983	20.3	108.7	18.7
1984	27.3	125.7	21.7

There is and will continue to be a strong demand for the construction of additional large facilities or the upgrading of existing ones. In view of the large and rapidly increasing fraction of the total DOE materials research budget devoted to the support of such facilities, the Board is concerned about the continuing support of the activities funded by the rest of the Basic Materials Sciences budget.

The pressures on these other portions of the DOE Basic Materials Sciences budgets have likewise increased. Inflation has squeezed operating funds, salaries, and equipment. The areas of responsibility for basic research have broadened as the responsibilities for support in materials science have moved from atomic energy to cover all energy sciences. In the universities, the need to upgrade research equipment in the laboratories of established individual investigators has become critical. Moreover, the increasing sophistication of equipment needed at the forefront of materials science has greatly escalated the cost of upgrading research equipment of materials scientists both in the national laboratories and in the universities. The problem is particularly acute for a new investigator.

The acquisition cost of some instruments is so large (between $250 thousand and $1 million) that these instruments are normally acquired for group use. Examples of such instrumentation are scanning transmission electron microscopes, scanning Auger spectrometers, secondary ion mass spectrometers, molecular beam epitaxy systems, ion implanters, and Rutherford backscattering spectrometers, to name but a few. Because the operation of these sophisticated instruments is complex, technical support staff are normally required for maintenance and operation. Thus, this type of instrumentation has effectively evolved into a "small" facility operation. At present the needs and costs of small facilities by the materials research community are also increasing at a rapid rate. It is understood that the Office of Energy Research has recently begun to address these needs. The Board encourages the continuation of these efforts.

Recommendations:

Because expenditures for construction or upgrading of large facilities frequently are justified by needs of potential users outside DOE materials programs, their funding should include appropriate additions to the BES materials budget. The additions should include the cost of operation. DOE should formally review large facility needs periodically, and when large facilities become outmoded, they should be shut down promptly.

The Director of Energy Research must have a strong role in working with other administrators in DOE to develop means or procedures to maintain a proper balance between expenditures for large facilities and those for the rest of the DOE materials science program and thus to prevent the large facilities from having a negative impact on the rest of the program.

C. Are the responsibilites assigned to the nondefense laboratories adequate to allow the effective development of relevant materials programs?

Findings:

To address the charge of whether "DOE energy and defense systems materials needs [are] being effectively translated into materials research programs and directed toward solving these specific problems," the responsibilities of the DOE laboratories must be delineated. For some of the energy laboratories, the development and management of unique large facilities along with the concomitant research constitutes their principal responsibility. In general, the laboratories should have the stability in responsibility and funding necessary for attacking and solving major long-term problems.

When the various DOE laboratories were founded, each laboratory was charged with a specific responsibility. For example, Oak Ridge National Laboratory was founded to solve the problem of the production and separation of plutonium on a time scale to meet the needs of the Manhattan Project. Similarly, Argonne National Laboratory had a responsibility for reactor development.

In viewing DOE laboratories today, the Board finds that generally defense systems materials needs are being met effectively through appropriate assignment of systems development and engineering responsibilities by DOE to the laboratories. In addition, the laboratories have been given sufficient authority and funding flexibilities to carry out these responsibilities. In this framework, there has generally been excellent continuity in the flow of materials innovations from the stages of research to engineering and the integration of these innovations into weapons design.

The Board finds that the nondefense energy laboratories are not fully effective in translating DOE energy systems materials needs into research programs directed toward solving pressing materials problems or incorporating the results into energy developments. The Board feels that this lack of coupling is in large part due to inadequately defined laboratory responsibilities. A clear-cut delegation of primary responsibility for some energy-related system, technology, or facility is essential if the energy laboratories are to provide strong direction to materials programs, couple materials programs adequately to applications, and maintain the correct balance between needs-oriented and opportunities-oriented research. Clear-cut energy responsibilities do not exist in this sense for the nondefense energy laboratories, and their absence adversely affects the conduct of materials R&D programs.* Underlying these concerns is a conviction that role statements and summaries of work programs do not substitute for clear-cut assignment of responsibility in energizing and giving direction to materials research programs. The Board notes that many of the nondefense energy laboratories have a stated responsibility for fundamental energy sciences, but it considers that these loosely stated responsibilities by themselves do not constitute useful guidance to materials research programs distinct from those conducted in universities.

The Board also notes that several of the nondefense energy laboratories have responsibilities for development and management of National Trust or other unique facilities such as advanced neutron and X-ray sources. The Board recognizes that these well-defined responsibilities, along with the concomitant research necessary to maintain expertise in the field, should in some cases constitute the principal mission of the laboratory.

The Board finds that primary authority for guidance and coordination of energy programs appears to reside in the Offices of Nuclear Energy, Fossil Energy, and Conservation and Renewable Energy, although some authority for particular task areas is often subcontracted to "lead laboratories." These lead laboratory assignments generally delegate responsibility, but little authority, for only a fraction of the total program and constitute only a small part of the total programmatic responsibilities of the laboratory involved. The Board does not consider lead laboratory assignments of this kind an adequate substitute for integrated responsibilities of the kind described above.† The lack of well-defined responsibilities and authority is particularly serious in areas such as coal liquefaction where there is a projected need for advanced energy technology but where no commitment has yet been made by government or industry to the engineering of prototype or commercial-scale systems.

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*Strong concerns about the problem of unclear missions was expressed in the letter of April 5, 1983, to J. Peter Grace from John Hanley and Roger Milliken (Ref. 5, p. 9). The same strong concern was expressed in the ERAB report of September 1982, The Department of Energy Multiprogram Laboratories (Ref. 6).

†This identical concern is expressed in the ERAB report The Department of Energy Multiprogram Laboratories (Ref. 6, p. 3).

Administration of most energy programs is widely dispersed, with responsibility for the conduct and planning of materials R&D often divided among the Offices of the Assistant Secretaries, the Energy Technology Centers, the Operations Offices, the lead laboratories, and the various R&D performers. Such widely dispersed authority and responsibility leads to inefficiencies in the operation of the materials R&D programs.

This lack of well-defined delegation of authority and responsibility to the energy laboratories has resulted in the lack of well-defined research priorities and thus in a nonoptimal allocation of resources. In this connection the Offices of the Assistant Secretaries for energy programs and the Director of Energy Research have been criticized for micromanagement of certain laboratory programs.* New arrangements for the support of materials research programs at the energy laboratories are needed to better define research priorities. In seeking these new arrangements, the Board emphasizes the importance of continuity of programmatic responsibility and level of funding appropriate for the achievement of desired technological goals.

Some DOE defense laboratories (Sandia, Los Alamos, and Livermore), have a practice of designating independent supporting R&D funds for applied defense missions. This practice has facilitated the coupling of basic materials science results to support mission objectives. The Board strongly supports this approach of providing independent R&D funds to the laboratory management of the nondefense energy laboratories.

Recommendations:

To improve the national focus on identification, conduct, and application of materials research and technology programs needed for future energy systems in the areas of Nuclear, Fossil, and Conservation and Renewable Energy, the Assistant Secretaries for these areas should develop a stronger focus within their offices and delegate broader responsibilities to energy laboratories than is now done under current DOE policy on lead laboratories. These assignments should focus on some energy system or technology, such as coal conversion or breeder reactors, and should include overall system responsibilities.

In the management of materials research at the energy research laboratories, DOE program managers should concentrate on defining areas of energy system relevance and need and on maintaining budget accountability. Within agreed-upon budget levels, the detailed management of materials programs should be the responsibility of laboratory directors.

The practice of designating independent supporting research and development funds for defense programs should be extended to the nondefense multiprogram energy laboratories to provide broad basic

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*This point has also been emphasized in the letter of April 5, 1983, to J. Peter Grace (Ref. 5).

materials support of their applied energy programs. The amount of such funds awarded should be appropriately related to the in-house applied program, decided on a case-by-case basis. Planning and implementing these programs should be primarily the responsibility of local laboratory management.

D. Are there important gaps in the DOE materials programs?

Findings:

The Board does not find that substantial opportunities in materials research are currently being overlooked. However, it does find a gap between materials research and materials engineering. The lack of attention given to materials technology development constitutes a programmatic gap in most nondefense DOE programs. The general function of technology development programs is to produce technology that provides at least one feasible alternate option, preferably more, for carrying out desired system functions. With respect to materials, this calls for a vigorous effort to generate both broad applied materials expertise and specific new materials capable of applications in realistic technological environments (as distinct from scientific sample generation, for example).

Materials innovations that have been reduced to practice at DOE laboratories are few. Development of new materials to the point where industry can produce them for application in energy systems usually requires several years and millions of dollars, especially if the application is in a nuclear system or requires American Society of Mechanical Engineers (ASME) Code approval. For example, development of modified 9 Cr-1 Mo steel to the point of application for ASME Code approval has required about seven years and more than $5 million.

Some organizations in DOE already have people assigned to work of this general sort (Development and Technology in Magnetic Fusion Energy, Advanced Research and Technology Development in Fossil, and Energy Conversion and Utilization Technologies in Conservation), but the function in general is not adequately recognized in organizational terms. For example, funds are often dispersed among the various system program divisions. Such an arrangement tends to cause the work to be done in a "firefighting" mode in the system test phase of the innovation process. Although working in such a mode is essential at times, the central need is for work done much earlier when more options and the possibility of coordinating the needs of different systems can be considered.

Such technology development programs will take advantage of the strengths of different groups of people and different institutions. In particular, while these programs need contributions from both universities and national laboratories, they are also natural points for industry contributions in the early phases of the innovation process. It is also likely that industrial participation at this stage will help with technology transfer.

Recommendations:

For each Assistant Secretary DOE should provide a needs-oriented technology development program with substantial materials elements. This could be done in the framework of a large transfer of responsibility to the laboratories (including subcontracting to industry and universities), which could find such programs supportive of their concept of the innovation process in general. If these programs are to succeed, the Board feels, a thrust in materials technology development must come from the Office of the Assistant Secretary and must have continuity of funding.

Organizational elements that carry out such technology development programs should be funded in parallel with system development, analysis, and engineering — not under them. Specific funding must be allocated to these technology development programs to provide the independence necessary to complete the materials development to the point of readiness for system application.

E. How can the results of materials R&D programs be more effectively incorporated into energy developments?

Findings:

Materials programs funded by DOE have, as their ultimate goal, the transfer of discovery into the technology base important to future weapons and energy systems. Materials research within DOE also represents an important source of new discovery. Therefore, it is in the national interest that mechanisms exist for both weapons and energy materials programs to promote and facilitate commercial exploitation.

Industry has traditionally provided the greatest momentum to materials innovation and application. The transfer to industry of emerging technologies and intellectual properties and their ultimate reduction to practice have been very effective where user needs have been clearly delineated.

Certain universities have shown that they can be effective sources of commercially exploitable discoveries. It is clear that technology transfer is possible and that successful universities should be studied to ascertain what qualities make them successful. A number of states are searching for mechanisms to use their university and research base effectively to promote the creation of new business.

Generally, DOE weapons laboratories have been effective in applying the results of materials research to systems production. This is largely due to the closed development cycle between DOE weapons laboratories and weapons contractors. The laboratories play a key role in engineering review prior to release for production, and the contractors depend upon the laboratories for the advanced developments of new weapons systems.

Such interdependent relationships between energy programs at the DOE laboratories and industry are spotty at best. DOE energy laboratories have been constrained in the past from having an open and businesslike relationship with industry. Furthermore, the dual roles of some laboratories as both developers of new energy technologies and suppliers of regulatory technical support in these technologies have caused industry to be wary and distrustful. Therefore, technology transfer from DOE laboratories to industry, which is difficult under the best of circumstances, has been further hampered by institutional and policy constraints. As a consequence, the number of successful technology transfers out of the DOE energy materials research programs has been disappointing.

Most patents derived from laboratory discoveries represent raw technology that must be further refined and tailored to market needs to become commercially viable. Industry requires adequate protection of developments during these risk-reduction stages to recover investments associated with commercialization.

The problems and barriers to technology transfer should not be minimized. The process is very difficult and requires a total commitment of the organization.

Recommendations:

DOE must provide clearly defined incentives for industry to show greater initiative in undertaking the process of technology transfer. Such incentives must include some form of protection to the company to justify the risk associated with commercialization of a new material. Increased emphasis on recently instituted arrangements for exclusive licenses or exclusive working arrangements that provide a head start should be employed to facilitate the transfer of technology from the laboratories to the marketplace.

DOE should seed materials research programs at selected universities, which would also draw heavily on state and/or industrial support, to promote technical innovation and proliferation of entrepreneurial companies.

Management of national laboratories should be evaluated in part on their success in promoting technical innovation and technology transfer. They should be encouraged to improve the environment for practical innovation and risk taking and to reward researchers who place a high value on innovation and reduction of technology to practice through a variety of channels.

DOE should pursue a more aggressive program aimed at identifying current and future directions in energy-related materials research carried out in foreign laboratories and to assess worldwide technology trends in energy materials.

VI. REFERENCES AND BIBLIOGRAPHY

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4. Energy Materials Coordinating Committee - Fiscal Year 1982 Annual Technical Report, DOE/FE/0033, March 1983.

5. Letter, from John Hanley and Peter Millikan to J. Peter Grace, April 5, 1983.

6. The Department of Energy Multiprogram Laboratories, a report of the Energy Research Advisory Board to the United States Department of Energy, DOE/S-0015, September 1982.

APPENDIX A

DEPUTY SECRETARY'S CHARGE

Department of Energy
Washington, D.C. 20585

November 2, 1982

Mr. Louis H. Roddis, Jr.
Chairman
Energy Research Advisory Board
110 Broad Street
Charleston, South Carolina 29401

Dear Lou,

As you are aware, the performance of materials is central to the economics, reliability and operational effectiveness of our existing energy production and conversion systems, and demanding materials requirements arise in the development of all new alternative energy technologies. In consequence, materials R&D is a major area of focus for DOE both from the standpoint of strengthening the science and technology base and from the standpoint of the development of component and systems technologies across all our R&D programs, with a present level of effort of over $275 million excluding classified materials R&D under the DOE defense programs. In addition, there are sizeable materials research efforts revelant to the energy mission sponsored by other Federal agencies and underway in private industry.

In its report on Federal Energy R&D Priorities, the Board gave the Materials Sciences highest priority among Science and Technology Base programs and materials research needs have been identified in various other ERAB studies. In view of the importance of materials to the improvement of energy technologies and their crucial role in the development of new technologies, it would be desirable for the Energy Research Advisory Board to undertake a review that would help the Department ensure that our programs are pursuing appropriate research goals and that effective interfaces exist with other agencies and the private sector.

In particular, I would hope that the ERAB study could consider these key questions:

- Are DOE energy and defense systems materials needs effectively translated into materials research programs and directed toward solving these specific problems and are the results of these materials programs adequately incorporated into energy developments?

- Are there important new opportunities in materials research that have been overlooked or are not being adequately addressed by DOE materials programs or elsewhere?

- Is the coordination and coupling of materials research programs between Government, national laboratories, universities and industry effective with respect to resource allocation and utilization of results?

- What is the significance and role of the DOE materials science programs relative to the Nation's overall effort in materials R&D, especially with respect to the development and support of major materials research facilities; how can the national contribution and benefits from DOE materials science programs be further enhanced?

In order to contribute to the Department's FY 1985 planning process, a report would be useful by August 1983 and, in any case, a final report not later than November 1983.

I appreciate the willingness of the Board to assist us in improving the Department's efforts in this important area.

Sincerely,

W. Kenneth Davis
Deputy Secretary

APPENDIX B

BOARD MEETINGS AND SITE VISITS

1983 MEETINGS OF THE ENERGY RESEARCH ADVISORY BOARD
MATERIALS R&D PANEL

Date	Purpose of Meeting
January 13	Briefings by DOE program staff on the Department's materials R&D programs
February 25	Briefings by Department of the Interior and National Science Foundation staff on their materials R&D programs
March 31	Briefings by Department of Defense and National Aeronautics and Space Administration staff on their materials R&D programs
April 11	Panel discussion of draft report outline
May 18	Reports on site visits and discussions of draft report outline
June 27–28	Reports on site visits and discussions of draft report sections
July 21	Discussion of draft report
September 12	Discussion of revised draft report (incorporating ERAB members' comments)
October 7	Discussion of final draft report

B-3

1983 SITE VISITS BY MEMBERS OF THE ENERGY RESEARCH ADVISORY BOARD
MATERIALS R&D PANEL

Date	Site
April 13	Brookhaven National Laboratory
May 13	Oak Ridge National Laboratory
May 16	Lawrence Berkeley Laboratory
May 17	Argonne National Laboratory
May 25	Lawrence Livermore National Laboratory and Sandia National Laboratory, Livermore
May 26	Los Alamos National Laboratory
May 27	Sandia National Laboratory, Albuquerque
June 24	Chicago O'Hare with University representatives

STATEMENT
ON THE
FY 1985
AUTHORIZATION
FOR THE
DEPARTMENT OF ENERGY
SUBMITTED TO THE
SUBCOMMITTEE ON ENERGY DEVELOPMENT & APPLICATIONS
OF THE
COMMITTEE ON SCIENCE AND TECHNOLOGY
U.S. HOUSE OF REPRESENTATIVES
BY

ROBERT M. ROSENZWEIG
PRESIDENT, ASSOCIATION OF AMERICAN UNIVERSITIES
ALSO ON BEHALF OF
THE NATIONAL ASSOCIATION OF STATE
UNIVERSITIES AND LAND-GRANT COLLEGES

MARCH 16, 1984

Mr. Chairman and Members of the Committee, my name is Robert M. Rosenzweig and I am President of the Association of American Universities. I submit this testimony in behalf of the membership of the Association of American Universities and the National Association of State Universities and Land-Grant Colleges which together represent 170 of the Nation's universities and colleges which carry out research supported by the Department of Energy. They also train almost all of the research scientists who carry on basic and applied research activities, not only at American universities but throughout American industry. As such, they together comprise the academic base for most of the Department of Energy's research and training programs. I would like to present to you our views with regard to the FY 1985 budget request for DOE university research and related programs by first addressing some general concerns and then discussing them in the context of the DOE budget.

General Discussion

All of our national policy objectives depend heavily on graduate education, both for highly trained personnel and for advances in scientific and technical knowledge that sustain our economy and ensure our defense. It is our graduate schools which provide the continuing supply of talented individuals with the knowledge, technical skills and perception which equips them to meet the challenges of this complex and and technologically sophisticated age.

We can look at our nation's modern history for evidence of this. During World War II, there was an emphasis on federal support for university programs for research and graduate training when there was a sudden dependency on university-based science and scientists. And again, in the late 1950s, after the successful launching of Sputnik, there was an increased federal interest and investment in research and advanced education as parts of a greater national effort to regain and sustain American scientific and technological superiority.

This led to a clear federal commitment to excellence in higher education and research. This manifested itself in the many programs of the National Science Foundation and the mission agencies, including NASA and the DOD, which contributed to strengthening our research and graduate education enterprise.

Since that time, the federal government has remained the primary patron of science. However, its investment in those core programs designed to strengthen graduate education and contribute to the research and education environment in universities has diminished significantly in some important areas.

The Department of Energy FY 1985 budget request proposes a 24% increase for basic energy sciences (+$82.2 million) and a 16% increase for general science (+$104.8 million). This represents a stronger commitment, and we hope it will be a sustained commitment, by DOE to its vital, but often neglected, fundamental research programs. The university plays a unique and essential role in the Department's research effort and its continued health requires a sustained national investment.

Today many of our leading graduate schools are seeing graduate enrollments tumble as undergraduate students clamor for the limited spaces available in our schools of engineering and computer science. The quality of instruction is being threatened. Faculty are strained to meet the demand, often without adequate assistance. More worrisome is the awareness that the ranks of truly talented young faculty coming along behind them are thinning. Time to pursue research frequently is squeezed, and the questions researchers are able to pursue in their investigations often are circumscribed by the obsolete instruments available to them. The capacity of faculty to substitute ingenuity for modern research tools is diminishing in many laboratories. In addition, many laboratories are aged; they require modernization if they are to serve through the decade as effective sites for the conduct of modern research. But, despite all of this, it is true that excellent research and quality education programs do continue in many laboratories. Many of those closest to the scene know, however, that increasingly serious problems do plague our research enterprise, problems that, left unaddressed, will compromise our future.

Recently, there has been recognition in many sectors including the Congress that indeed the quality of the environment for academic science and graduate education has suffered prolonged erosion. In fact, Majority Leader Jim Wright and some of his colleagues intend to introduce legislation which would implement a comprehensive plan to restore the research capacity of our nation's colleges and universities. The plan would provide for a broad federal investment in the major research agencies to strengthen the university-based research capability and graduate education programs.

Similar legislation, The University Research Capacity Restoration Act of 1983 (S.1537), was introduced in the Senate last year. That bill sets an agenda for a five-year program of increased federal support in the six major research agencies: (1) to augment and strengthen federal support for fundamental research programs in basic science and engineering at the nation's universities; (2) to upgrade and replace the instrumentation and equipment of university research facilities and laboratories; (3) to provide increased numbers of graduate fellowship awards to individuals and university departments engaged in federally supported research; (4) to support expanded faculty development programs that promote the initiation of research careers by young university faculty; (5) to support efforts, on a matching basis with the institution involved, to

rehabilitate, replace or otherwise improve the quality of existing university research facilities and laboratories in which federally supported science and engineering research is carried out; (6) to modernize and improve undergraduate science and engineering instructional programs and curricula to meet the nation's changing needs.

We congratulate the sponsors of these initiatives and ask that this Committee seriously consider the Wright proposals when they are introduced.

I would like to address five areas which are appropriately considered in the context of the FY 1985 DOE budget request: basic energy science research programs, graduate student support, career enhancement initiatives for young faculty, research instrumentation and research facilities.

Basic Research Programs

The proposed budget for Basic Energy Sciences is $82.2 million (24%) higher than the current level. This budget will provide needed continuity for the various science programs including a significantly enhanced materials sciences program. It will also fund a new effort by the Department to provide access to supercomputers for researchers. The proposed General Science budget is $104.8 million (16%) higher than the current level. These programs support important long-term basic science research in the areas of High Energy Physics and Nuclear Physics. The budget also will provide essential support to modernize several accelerators and research projects.

We commend these proposed increases. In recent testimony on the FY 1985 DOE budget request before the House Appropriations Subcommittee, Dr. Alvin W. Trivelpiece stressed that these research programs often involve the training of graduate students at universities that have made significant contributions to the economic growth and prosperity of the nation. It is precisely for this reason that we ask the Committee to authorize an additional $20 million for the basic energy sciences programs at universities for investigator-initiated fundamental research.

Graduate Education

In 1968, 51,000 federally funded fellowships were awarded. Today fewer than 10,000 are awarded and of these, only 1,500 are awarded to students in advanced study in the sciences and engineering. DOE awards only about 25 such fellowships in narrowly defined fields. We previously have asked the Committee to review the problem of shortages of support for graduate students in energy-related fields. In the recent past, this Committee did respond by authorizing a small graduate traineeship program, but it failed to be enacted. We understand that the Department of Energy attempted again to implement a graduate fellowship program for FY 1985, but it reportedly was not supported by the Office of Management and Budget. It is

unfortunate that these attempts have failed. We believe that this Committee's attempt to strengthen DOE's commitment to graduate education continues to be worth the effort. We urge you again to consider the need for a DOE graduate fellowship program.

The best approach, we respectfully suggest, would be a two-part program, each funded at $2.5 million, to provide for (1) merit-based, portable, three-year graduate awards to students and (2) a comparable number of awards to departments that carry out DOE-funded basic research programs. The positive implications for the health of science and engineering departments doing energy-related research would be very great, while significant numbers of students would be assisted toward completing their studies. Both the National Science Foundation and the DOD's Office of Naval Research have strong merit-based, portable graduate fellowship programs in place. The ONR graduate fellowship program is the present model for excellence. It provides a stipend of $13,000, full tuition, plus $12,000 research award to the host department. We recommend that DOE implement a program fashioned after it.

Young Faculty

Increasingly serious challenges face young researchers who seek to begin careers in basic science. Young Ph.D.s who complete their formal training and aspire to academic careers face hurdles more serious than those their faculty mentors encountered. The attractiveness of an academic career is diminished and the prospects for a successful start need enhancing.

The 1982 AAU report to NSF, "The Scientific Instrumentation Needs of Research Universities," provides a striking example of the increased costs young researchers face as they seek to establish their research programs. The data now are somewhat dated, so the message they convey should be interpreted as a conservative estimate of the present cost. In the case of a leading chemistry department the costs associated with equipping a new faculty member to do up-to-date research in the field of synthetic organic chemistry increased from $116,500 in 1970 to $741,000 in 1979. Inflation accounts only for part of the rising costs. Imposed on the rising baseline of inflation are the much larger costs resulting from advances in existing instrumentation and the development of totally new, more powerful, and, therefore, more productive instruments. Young researchers of promise, but who are yet without successful track records, cannot meet these costs without substantial assistance from their departments and institutions; and they are increasingly hampered in being able to respond.

The National Science Foundation has instituted a new program to provide recent Ph.D.s with five-year awards averaging $30,000 to be matched by private sources. These awards would enable the young faculty member to begin research immediately, with an opportunity to develop skills in the early years of his career.

For some, it will mean the difference between remaining in the academic environment and leaving to pursue more encouraging and fruitful alternatives.

The Department of Energy should be encouraged to start a comparable program targeted on enhancing the human resource pool in energy-related fields. An initial investment of $5 million would start this initiative in FY 1985.

Research Instrumentation

The budget requests $6 million to continue the essential effort to upgrade university research instrumentation and equipment, started by DOE in the current fiscal year (FY 1984) at $4 million. We commend the Department for doing its part to address the needs of obsolete university research instrumentation and we fully support the effort. We encourage the Committee at a minimum to support DOE's program for university research instrumentation in FY 1985. Beyond that we ask that the authorization for this program be revised by $24 million, to $30 million per year. This would fund the effort at a level equal to DOD's research instrumentation program.

I should like also to take this opportunity to tell you about a new research project, now being undertaken by three higher education associations with the support of NSF, DOE, and several other agencies, to explore alternative solutions to the equipment problem. The project is seeking to identify and to evaluate new approaches to acquiring, managing, and using equipment and to inform the university community and others of the results of these evaluations. It is a joint undertaking of the AAU, the National Association of State Universities and Land-Grant Colleges (NASULGC), and the Council on Governmental Relations (COGR). The project is being supported jointly by the Department of Energy, NSF, NIH, DOD, USDA, and NASA. The Research Corporation also has made a contribution. The effort is being carried out under the guidance of an eight-member steering committee drawn from universities, industry, and the national laboratories. A list of steering committee members is attached (Attachment A).

The project grows out of a 1980 AAU report NSF titled The Research Instrumentation Needs of Universities. That report documented the dimensions of the equipment problem in 15 leading universities by comparing their research equipment holdings with the equipment used in a number of leading commercial laboratories and major national laboratories. As shown on the attached graph (Attachment E), the median age of the equipment in the universities was found to be twice that of equipment in the commercial laboratories. The executive summary of the report is attached to my statement (Attachment C). The complete report was submitted to the Committee in an earlier hearing.

As new investments in research equipment are made by DOE and by other agencies, we also must explore for new approaches to help ensure that our investments yield the maximum scientific and technological return.

Recognizing this fact, the National Science Foundation asked AAU, NASULGC, and COGR to convene an ad hoc planning committee to consider whether a special effort was needed to explore ways to improve the acquisition, management, operation, and maintenance of equipment. The group identified the following questions:

1. Does so-called debt or creative financing hold significant untapped potential for universities as a means of financing new research equipment?

2. What more can universities do to improve the way they acquire, manage, and use research equipment?

3. Can innovations made by government and commercial laboratories be identified and adapted for use by universities?

4. Are there regulatory and policy barriers in universities or the states that can be identified and steps that can be taken to remove or reduce them?

5. Can present tax incentives for the donation of research equipment be improved to increase support from industry?

6. Are there changes that ought to be made in federal regulations that would ease the situation?

7. Are there alternative methods of direct federal funding that would yield a better return on federal investment?

PHASE I

The project began last November. It is scheduled to be completed in February, 1985. The work is planned in three phases. During Phase I analyses will be conducted in six areas:

1. The first is the role of debt financing of research equipment in sound university financial practice.

   Considerable attention is being paid in some parts of the research community to developing new, creative modes of financing the acquisition of university research equipment. The potential usefulness of such approaches is being debated intensely, but the techniques themselves often are not well understood, and experience in their use varies considerably. This analysis will identify the

various methods of debt financing. It will assess the desirability of encouraging deeper involvement by universities in their use, give the pros and cons of different financing approaches, and provide examples of what has worked, where these techniques have worked and why. The analysis also will offer suggestions to help institutions evaluate the appropriateness of these approaches in the light of their particular circumstances.

2. The procurement, management, and use of research equipment is the subject of the second analysis.

Opportunities to strengthen the organization and management of university laboratories and supporting services will be identified and assessed by the second analysis. Particular attention will be paid to new methods of sharing equipment among departments and universities. This analysis will identify barriers to sharing inherent in the nature of university research and will consider possible ways to lower such barriers. Recent experience in using advanced technology to provide remote access to high-cost equipment will also be examined. Finally, the management practices of selected commercial and government laboratories will be reviewed to seek approaches that might be adapted to the university setting.

3. The third analysis will assess tax incentives for the donation of equipment and suggest ways to increase support from the private sector.

The Economic Recovery Tax Act of 1981 provided new incentives designed to stimulate donations of equipment to universities by industry. Experience to date seems to indicate that this provision is having a significant and beneficial impact on the problem. This analysis will evaluate the experience to date and assess opportunities to strengthen further this new incentive to corporate support.

4. Reduction of regulatory and policy barriers in states and universities is the subject of the fourth analysis.

A selected number of state governments and universities will be surveyed to determine whether there are policy and regulatory barriers to improved acquisition, management, and use of research equipment. Particular attention will be given to provisions in state constitutions and laws which may restrict university efforts to improve their research laboratories. Some states, for

example, have laws that inhibit greater use of creative financing techniques by universities. This is a very complex and difficult arena. But we do hope to identify such barriers and to formulate proposals for improvements or changes that might be considered by state governments and their public universities.

5. In the fifth analysis federal regulations governing the acquisition, management, and use of equipment will be reviewed.

Recommendations will be made for changes to current regulations that would facilitate equipment acquisition, achieve management improvements, and ease burdensome reporting requirements.

6. The subject of the sixth analysis is future methods of direct federal investments.

The current methods or means of federal funding of research equipment will be evaluated. The benefits and limitations of these methods and the pros and cons of changing them will be assessed. Alternatives will also be explored with an eye to maximizing the return to the nation of future investment of scarce federal resources. One option that will be explored is the feasibility of returning to the use of the proven but presently unutilized mechanism of guaranteed loans to rehabilitate university research laboratories and equipment. As the committee knows, in 1965 the Higher Education Act established a guaranteed loan program (Title VII-C) designed to assist with the rehabilitation of academic laboratories, and that program played a substantial leadership role in mobilizing other state, private, and institutional funds. For more than a decade, however, that loan program has not been funded. Reinvestment in the Title VII program is one option; others will be considered.

The project contracted with the accounting firm Coopers & Lybrand to do the research and analysis on several of the analyses: debt financing, tax incentives, federal and state regulations, and future methods of direct federal investment. The analysis of opportunities for improvements in university procurement, management, and use of equipment is being carried out by a team of three university people: David Litster, Director of MIT'S materials science center; Robert Bock, Dean of the Graduate School at the University of Wisconsin; and Julie Norris, Assistant Provost of the University of Houston. Over the next four

40-574 O - 85 - 96

months they will visit and gather information from 12 universities and 8 corporate and government laboratories.

PHASE II

During the second phase of the project, beginning in the fall of 1984, the results of the six analyses will be disseminated to the university community. Leading higher education associations and science and engineering societies will be invited to join the project as cooperating organizations, and to host special seminars as part of their regularly scheduled meetings. Regional workshops will be held in September and October 1984. They will be designed to provide opportunities for teams of representatives from universities in each region to share their varying perspectives on the equipment problem. During the workshops each team will be invited to explore the implications for their own institutions of adopting approaches identified by the Phase I analyses.

PHASE III

The project's final phase will be an agency briefing in Washington to report the results of the project to the sponsoring federal agencies and to the Congress. A final report will be submitted to the sponsoring agencies in January 1985.

OBSOLETE FACILITIES--THE OTHER SIDE OF THE EQUIPMENT PROBLEM

Any discussion of the research instrumentation needs of universities is incomplete if it does not also address the interrelated research facilities problem. Modern research instrumentation increasingly requires specialized environments, and many of our research laboratories are obsolete and inadequate settings for modern science. They often require extensive and costly modernization or replacement. It is noteworthy that the DOE has not only recognized, but is addressing, the serious problem in its own laboratories. Through the multiprogram, general-purpose facilities budget, the Department continues to rehabilitate and replace outdated facilities at its multiprogram sites.

The dimensions of the facilities problem are estimated to be considerable. In 1981, the AAU surveyed the facilities needs of 15 major universities. In FY 1979 these institutions accounted for about 22% of total federal obligations for university-based research. The scope of the survey included the needs of only present programs and faculty; planned new programs and new hires were excluded. It found these institutions able to meet only about half of their projected needs for replacement construction, modernization, repair and renovation, and high-cost equipment (items capitalized at more than $100,000). The report's executive summary is attached to my statement (Attachment D).

The facilities deficit is almost certainly the most serious long-range problem that now confronts our research universities and the agencies for which university researchers perform research. A recent survey by the University of California, for instance, found "staggering" facilities problems, including estimated needs for core academic facilities alone totaling $1.6 billion over the next decade. Traditional funding approaches, the university concluded, simply will not meet their need for facilities rehabilitation and replacement. Failure to address this backlog, however, will certainly result in compromised instructional and research programs.

We understand that the Department of Energy has joined with the Department of Defense and with other agencies in planning a comprehensive study of the problem. We are pleased indeed that the Department is participating to develop both a better understanding of the problem and suitable solutions.

We believe it is time for the leading agencies of the federal government that fund the nation's basic science programs to assist in the rehabilitation of those laboratories essential to each agency's research mission and goals. We ask that the committee consider establishing a program to rehabilitate DOE-funded university laboratories at a level comparable to the multiprogram, general-purpose facilities program--$40 million.

Recently the National Commission on Student Financial Assistance (a bipartisan panel created by P.L. 96-374, the education amendments of 1980) completed its report, "Signs of Trouble and Erosion: A Report on Graduate Education in America." The Commission affirms the seriousness of the instrumentation and facilities deficits and it calls for just such an investment strategy for research instrumentation and facilities rehabilitation as that proposed by S.1537 discussed earlier in this testimony. We commend that report to the Committee's attention.

A serious debate leading to concrete proposals for a facilities reinvestment strategy is needed. We hope that this committee will consider the facilities problem as part of its continuing deliberations on the research equipment problem and the FY 1985 Department of Energy budget request.

Peer Review

The future return on all of these essential investments, of course, will be determined in large part by the soundness of the decisions that the Congress and the Department of Energy make in the award of the funds. The funds ought to be awarded on the basis of scientific merit in open competition among all interested and qualified parties. Final judgments ought to be formed in an objective and informed manner, free from any actions by particular individuals or institutions that could serve to make the award of such funds a matter of political influence rather than the quality of the work to be done and the capacity of competing applicants to carry out the work at the highest level.

Recently the Association of American Universities, the American Council on Education, the National Association of State Universities and Land-Grant Colleges, and the Council of Graduate Schools joined others in addressing the importance of protecting and relying upon the established processes of informed peer review in the statements recently adopted by these associations are attached to my statement (Attachment B).

DOE-University Forum

Finally, Mr. Chairman, we are pleased to hear that in the next few months, the Department of Energy will establish a DOE-University Forum designed to foster a sustained dialogue on topics of mutual concern between the Department and our research universities. The effectiveness of the DOD-University Forum gives us hope that the DOE activity will be similarly useful.

We commend the Department for establishing the Forum, and we hope that the Committee will follow its activities with interest.

Thank you Mr. Chairman for the opportunity to present our views to the Committee.

ATTACHMENT A

PROJECT TO ASSESS & DISSEMINATE ALTERNATIVE APPROACHES TO MEETING UNIVERSITY RESEARCH EQUIPMENT NEEDS

Steering Committee

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ATTACHMENT B

AAU Association of American Universities

AAU STATEMENT ON DECISION MAKING IN FEDERAL FUNDING FOR RESEARCH FACILITIES

The Association of American Universities represents institutions whose faculties are deeply engaged in research. We share with many other institutions and individuals a commitment to advancing the quality of the nation's research effort. Since the vitality of this effort is closely linked to the soundness of decisions made about science by public bodies, it is both appropriate and important for the AAU to state its collective views about the ways in which those decisions are best made.

The United States has evolved an admirable but fragile system of awarding federal funds for research. In general, Congress appropriates funds for the support of broad categories of research. Subsequently, the administering federal agency issues guidelines for making applications in a manner that assures fair and open competition. Researchers then submit detailed proposals that are judged by experts, scientists chosen for their ability to make sound and careful judgments in the scientific area involved. This method maximizes the scientific return on the federal investment by assuring that awards are made on the scientific merit of the proposal and the professional merit of the proposer.

The same method governed most federal programs in support of scientific facilities when such programs existed. However, in the early 1970s, most federal government programs in support of the construction and renovation of research facilities ended. The subsequent decade-long failure to attend to the capital base of university science has led to a backlog of need that has hampered American science and placed great stress on the processes by which the government allocates scientific resources.

We believe that processes based on the informed peer judgments of other scientists need to be preserved and strengthened. We therefore urge scientists, leaders of America's universities, and Members of Congress to support the practice of awarding funds for the support of science on the basis of scientific merit, judged in an objective and informed manner. Further, we urge them to refrain from actions that would make scientific decisions a test of political influence rather than a judgment on the quality of the work to be done. These principles should apply in making decisions about scientific facilities as well as in awarding funds for research projects.

Finally, we urge officials of the national Administration and Members of Congress to deal promptly with the decay of the physical plant that houses much of the nation's basic research. S.1537, introduced by Senators Danforth and Eagleton, is a bipartisan effort to deal with this national priority and deserves strong and prompt support.

October 25, 1983

National Association
of State Universities
and Land-Grant Colleges

Robert L. Clodius, President

STATEMENT ON FEDERAL FUNDING OF ACADEMIC FACILITIES

In recent years, federal funding of various higher education programs had decreased markedly. In particular, wholly inadequate resources for facilities has led some institutions to seek direct assistance from Congress. The outcome of such a process could be an irrational system of distribution based solely on political influence. In that regard, the National Association of State Universities and Land-Grant Colleges shares the concerns of the Association of American Universities, the National Academy of Sciences, and others, that this approach is unacceptable, in that it could diminish the capability of higher education to carry out its mission in education and research, and we urge Members of Congress and leaders of colleges and universities to refrain from this practice.

We further urge the Congress to fund Title VII of the Higher Education Act and similar programs in other agencies at reasonable levels, and to insure the systematic allocation of resources to satisfy pressing national concerns.

November 13, 1983

One Dupont Circle N.W. Washington D.C. 20036 202 293-7120

The Council of Graduate Schools in the United States
One Dupont Circle, N.W. Suite 430 Washington, D.C. 20036-1173 Phone: 202/223-3791

RESOLUTION NO. 1

RESOLUTION IN DECISION MAKING IN THE FEDERAL FUNDING FOR RESEARCH FACILITIES

WHEREAS the United States has evolved an admirable but fragile system of awarding federal funds for research, and,

WHEREAS this system is dependent upon fair and open competition responding to federal agency guidelines, and peer review judgment by experts in the scientific area to be studied, and,

WHEREAS this method of peer review has governed most federal programs in support of scientific facilities when and where such program exist, and,

WHEREAS most federal programs to support construction and renovation of research facilities have been ended through a shifting of federal priorities, and,

WHEREAS in the absence of such programs colleges and universities are suffering a gradual increasing erosion in their ability to support state-of-the-art research in all scientific fields, and,

WHEREAS CGS member institutions share with many other institutions and individuals a commitment to advancing the quality of the nation's research effort. The vitality of this effort is closely linked to the soundness of decisions made about scientific research by public bodies.

NOW THEREFORE BE IT RESOLVED that the Council of Graduate Schools supports the recently adopted AAU Statement on Decision Making in federal funding for research facilities. CGS urges the national Administration and members of Congress to support the practice of awarding funds for research or facilities on the basis of scientific merit judged in an objective manner. CGS would further urge support for new spending authorities to support research facilities to keep our nation's investment in academic research facilities from becoming out of date.

Passed at the CGS 23rd Annual Meeting 12/83

Affiliates:
Conference of Southern Graduate Schools
Midwestern Association of Graduate Schools
Northeastern Association of Graduate Schools
Western Association of Graduate Schools

Adopted at the Board of
Directors meeting of
2/23/84

Ruth A. Abdouch
Executive Secretary
Board of Directors

AMERICAN COUNCIL ON EDUCATION

5. Federal Relations Report
   B. Proposed Statement on Federal Funding of Research and Instructional Facilities

For Board Approval

BOARD OF DIRECTORS
Meeting of February 23, 1984
10:00 a.m.-3:00 p.m.
Kellogg Room
One Dupont Circle
Washington, DC

AMERICAN COUNCIL ON EDUCATION
Office of the President

MEMORANDUM

TO: ACE Board of Directors

FROM: J. W. Peltason

SUBJECT: Proposed Statement on Federal Funding of Research and Instructional Facilities

DATE: January 9, 1984

Community concern has been generated by the recent attempts of several institutions to bypass the customary review process to obtain federal funding for research facilities. The Association of American Universities last fall issued a statement urging scientists, leaders of America's universities, and members of Congress "to support the practice of awarding funds...on the basis of scientific merit...(and) to refrain from actions that would make scientific decisions a test of political influence rather than a judgment on the quality of the work to be done."

Similar statements have been issued subsequently by the National Academy of Sciences, the National Association of State Universities and Land-Grant Colleges, and the American Association of State Colleges and Universities. The ACE Commission on Governmental Relations discussed this matter at its fall meeting, and recommended that the Board adopt the following statement:

"There is a pressing need for increased federal support for the rehabilitation of research and institutional facilities. Established procedures for these support programs involve a system of review to assure equitable consideration and the awarding of funds on the basis of merit.

"At a time when fiscal constraints have severely restricted many federal programs, it is especially important to sustain the process which assures systematic allocation of scarce resources. Therefore we call upon leaders of the academic community and members of Congress to reaffirm the principle of broadly representative review of project proposals in fair and open competition, so that funding decisions continue to represent the best interests of both higher education and the national welfare."

One Dupont Circle, Washington, D.C. 20036-1193
President (202) 833-4710 Vice President (202) 833-4712

ATTACHMENT C

THE SCIENTIFIC INSTRUMENTATION NEEDS OF RESEARCH UNIVERSITIES

A Report to the National Science Foundation

by the

Association of American Universities

June 1980

The Scientific Instrumentation Needs of Research Universities

EXECUTIVE SUMMARY

OBJECTIVES OF THE STUDY

- assess the current status of scientific instrumentation in major research universities
- identify factors which facilitate or impede its development, acquisition, use, and maintenance
- estimate the future consequences of present funding policies
- recommend appropriate policy changes

METHODOLOGY

- sixteen universities, six national and government laboratories, and nine commercial laboratories were visited; about 80 department heads and over 250 researchers and research administrators were interviewed in the universities; in addition, the views of approximately 60 researchers and research managers were gathered in visits to national, government, and commercial laboratories
- five fields of science and engineering were studied: physics, chemistry, biological sciences, earth sciences, and electrical engineering
- numerical data on instrumentation acquisition, age, and replacement were gathered from 14 universities and four commercial laboratories

THE PROBLEM

Instrumentation is essential for progress in experimental research. Scientific knowledge has advanced rapidly; new instruments, more costly but qualitatively superior to earlier ones, have allowed measurements previously impossible. The rate of change has been great, competition among researchers intense. The capacity of university researchers to work at the frontiers of knowledge has important consequences for the nation's future research productivity and for the training of future generations of scientists and engineers.

The federal government has adopted a variety of funding policies for the support of research instrumentation: the competitive project system, special instrumentation programs, formula grant programs, block-funded centers, federally sponsored research centers, and regional instrumentation centers chief among them. For about 15 years, federal support for basic research has gradually declined; now support levels are further strained by rapid inflation. But inflationary price increases are simply the rising baseline upon which are superimposed the frequently much larger increases resulting from instrumentation advances.

ASSESSMENT

The great diversity of instrumentation needs found among institutions visited precludes simple generalizations. However, problems in the acquisition, use, and maintenance of research instrumentation were found in all of the leading universities visited. The precise configuration of these needs and problems varies widely. The capabilities of institutions and departments to meet them do also.

University researchers face great difficulty in replacing worn-out or obsolete instrumentation and in acquiring new instruments needed for frontier research. A comparison of university instrumentation inventories with those of two leading commercial laboratories reveals that the median age of university equipment is *twice* that of the commercial laboratories' instrumentation. Even the nation's major research universities have not kept pace in meeting instrumentation needs. Researchers heavily dependent upon federal funds have witnessed grant size fall behind escalating research requirements. As a result, many work with inadequate tools that impair the pace

of research, force closure of lines of inquiry, strain operations and maintenance budgets, and compromise the advanced education of graduate students.

Start-up funds for new faculty often are shrinking as costs rise. Support equipment is needed to test, calibrate, and augment primary instruments. Often it is especially difficult to fund. Funding for operation and maintenance costs is increasingly difficult to obtain. As a result, faculty and students sacrifice research time to these routine tasks.

Many research facilities are in need of renovation or replacement; federal funding for these purposes has decreased, however, and universities lack the funds to respond. Signs that aging facilities now impede research were found in many laboratories and support facilities.

Local university needs vary widely, reflecting the unique circumstances under which each institution operates and the great diversity between and even within the five fields studied. Present funding policies do not provide sufficient flexibility to deal with such local circumstances.

When compared with government and commercial laboratories visited, most university laboratories fare poorly. The best-equipped industrial laboratories surpass almost all university laboratories visited. One university researcher captured the sense of disparity and observed, "the ivory towers are now in industry." The director of one leading industrial research laboratory described the struggle of university researchers as he has observed them as "pathetic." When asked to contrast their laboratories with foreign laboratories, a number of university researchers stated that many, most notably those in Japan and West Germany, are now superior.

CONCLUSION

The quality of research instrumentation in major university laboratories has seriously eroded. Not all, but many researchers in the nation's best-funded universities are struggling to work effectively with obsolete tools. The equipment being used in the top-ranked universities has a median age twice that of the instrumentation available to leading industrial research laboratories.

Three *causes* are identified:

- a relative decrease in instrumentation support
- inflexibility within the project system
- insufficient support for maintenance

Three major *consequences* are:

- diminished research productivity
- reduced training capacity
- decline in international competitive status

RECOMMENDATIONS

Federal policy for the support of research instrumentation should provide for a basic three-part funding strategy:

- strengthen instrumentation funding in the project system
- expand special instrumentation programs
- create in the National Science Foundation a new, supplemental formula grant program to provide needed flexibility to meet diverse institutional needs

FUTURE STUDIES

Five studies are recommended: 1) a thorough analysis of foreign research funding policies and programs and their implications for the competitive stature of American science should be undertaken; 2) a study of cooperative research arrangements between industries and universities and the factors—including federal policies—that encourage and discourage them is needed; 3) the planned assessment of regional instrumentation centers should include consideration of the concerns documented in this report; 4) universities should assess current instrumentation policies and develop mechanisms and incentives designed to promote effective sharing of instrumentation; 5) an assessment of the costs and benefits of federally-mandated equipment inventory and reporting systems should be undertaken.

ATTACHMENT D

THE NATION'S DETERIORATING UNIVERSITY RESEARCH FACILITIES

A Survey of Recent Expenditures and Projected Needs in Fifteen Universities

July 1981

Association of American Universities
One Dupont Circle, N.W.
Washington, D.C. 20036

EXECUTIVE SUMMARY

OBJECTIVES OF THE SURVEY

This survey of 15 leading universities had three objectives:

-- In the institutions surveyed, document expenditures for research facilities and major ($100,000 or more) equipment, without regard to source of funds, over the last four years in the following six fields:

- Biological Sciences
- Chemical Sciences
- Earth Sciences
- Engineering
- Physics
- Medical Schools (10)

-- Provide responsible estimates, prepared by those universities, of expenditures for research facilities and major equipment that would be required over the next 3 years to meet the research and training needs of only current faculty.

-- From researchers and department heads, acquire assessments of the major consequences for science, industry, and government if the accumulating facilities needs of their institutions are not addressed.

FINDINGS

In many of the science and engineering departments surveyed, a substantial backlog of research facilities and equipment needs is accumulating. Projected funding needs over the next three years equal almost twice the level of expenditures by universities for their research laboratories and equipment over the past four years. Already, institutions often are unable to provide their basic science and engineering researchers and students with either the modern laboratories or equipment needed to conduct state-of-the-art research and education programs.

The loss of federal contributions to the support of research facilities and the absence of compensatory sources of support has forced many institutions to renovate and repair only those facilities in greatest need. Even this work often is carried out in a necessarily piecemeal fashion which is uneconomical over the long term. Working under such conditions, researchers unavoidably compromise their productivity and future competitiveness.

Relatively few construction projects have been completed in recent years in a majority of the physical sciences and engineering departments surveyed. Many institutions estimate substantial needs for new laboratories, for the expanded modernization and repair of old laboratories and for modern research equipment. Details are provided in the following report and the appendicies. The survey's principal findings are the following:

- In the last four years, for the six fields surveyed, fifteen leading universities together spent $400 million from all sources for facilities and major equipment. Half of those expenditures was for a relatively small number of new construction projects; the remaining half, spread over a larger number of generally less costly funding projects, was for facility modernization, major repair and renovation, and special purpose research equipment.

- In the next three years, the 15 universities estimate they should spend almost twice as much ($765 million) just to provide the necessary research facilities and special research equipment for current faculty only. These estimates are in current dollars and, therefore, do not include the added effects of inflation.

- New construction to replace outmoded facilities accounts for almost 60% of total projected funding requirements across all fields.

- In addition, substantial needs for major research equipment were identified in all six fields. These equipment estimates include only major items costing at least $100,000. As the 1980 AAU report to the National Science Foundation found, most departments also have serious deficiencies of less costly analytical instrumentation and support equipment.

RECOMMENDATIONS

The problems of obsolescence in the nation's university research facilities have been growing for more than a decade. To solve them, a new national investment strategy is needed. That strategy should provide direct, balanced support for university facilities from federal agencies and provide investment incentives designed to involve industry, the states, and the universities in a coordinated effort. The following steps are suggested as starting points:

1. Key Executive agencies should develop a mechanism to periodically assess the condition of university research laboratories and the consequences for the nation of that condition. Such assessments should involve the Office of

Science and Technology Policy, the National Science Foundation, the Department of Defense, the Department of Energy, the Department of Health and Human Services, the Department of Agriculture and the National Aeronautics and Space Administration. The views of industry and the universities also should be solicited.

If the initial review corroborates the assessment of this suvey the following recommendations should be considered:

2. The facilities and equipment program earlier proposed to be undertaken by the National Science Foundation but deferred should be restored as a priority initiative in FY 1983.

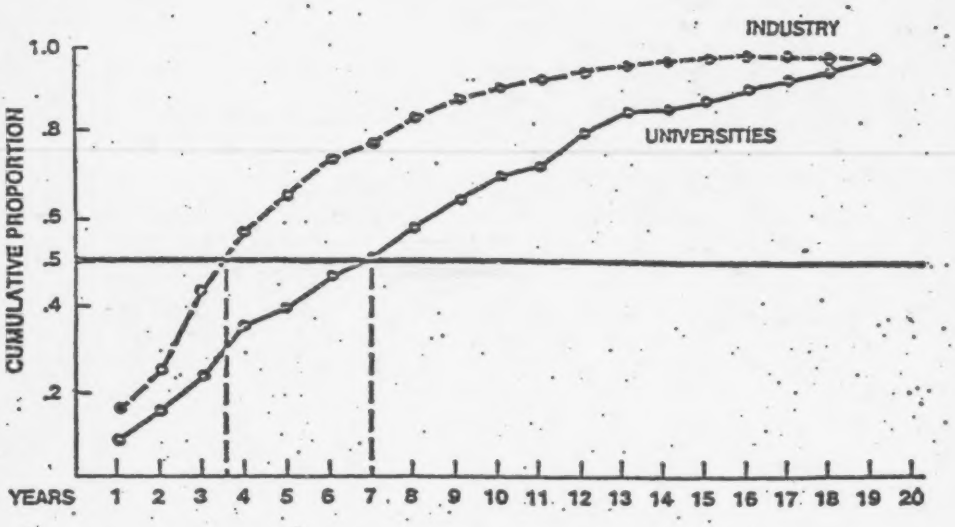
3. The Department of Defense, Department of Energy, the National Aeronautics and Space Administration, the Department of Health and Human Services, and the Department of Agriculture should establish research instrumentation and facilities rehabilitation programs targeted on the fields of science and engineering of primary significance to their missions. The National Science Foundation should assist in the development, implementation, and coordination of those activities.

4. Incentives should be provided to encourage industries and the states to join with universities and the federal government in renewing the nation's university research laboratories.

5. Interest costs incurred in the construction, modernization, renovation, and repair of facilities in which federally supported research programs are carried out should be allowable indirect costs under OMB Circular A-21.

ATTACHMENT E

Age of Instrumentation in Universities Twice That in Industry



DEPARTMENT OF ENERGY

FISCAL YEAR 1985 CONGRESSIONAL BUDGET REQUEST

ENERGY SUPPLY RESEARCH AND DEVELOPMENT

VOLUME 3

SUPPORTING RESEARCH AND TECHNICAL ANALYSIS

TABLE OF CONTENTS

Program Overview 143

Basic Energy Sciences 145

Energy Research Analysis 211

University Research Support 215

University Research Instrumentation 223

Advisory and Oversight Program Direction 227

Multiprogram General Purpose Facilities 229

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
PROGRAM OVERVIEW

Supporting Research and Technical Analysis

The need to develop new and improved energy sources and to use energy more efficiently continues to be extremely important to the general welfare of the Nation. The role of basic (or supporting) energy research and technical analysis is to expand the scientific and engineering knowledge base on which the Nation's future energy options depend and to provide independent, objective analyses and assessments of research and technical needs relating to energy. Funding of basic research is an investment in the future. Through this investment, the applied technology efforts of industry and government will have a broader foundation of knowledge from which to discover new concepts, materials, processes and techniques important for energy production, conservation and utilization. Failure to strengthen our fundamental knowledge base of energy-related phenomena could result in limitations on productivity growth, erosion of the country's competitive position with foreign nations, additional pressure on the United States balance of trade and continuation of inflationary trends.

The following seven programs comprise the Office of Energy Research's portion of the Supporting Research and Technical Analysis category of the agency's budget: (1) Basic Energy Sciences (BES); (2) Energy Research Analysis (ERA); (3) Advisory and Oversight Program Direction; (4) University Research Support (URS); (5) University Research Instrumentation (URI); (6) Multiprogram General Purpose Facilities (MGPF); and (7) Policy and Management. All seven of these programs are organizationally in the Office of Energy Research.

The Basic Energy Sciences program is responsible for the long range, basic research of the agency to provide the fundamental scientific and engineering base on which the Nation's future energy options depend. The major product of the BES program is increased knowledge. This knowledge is developed by sponsoring research in the traditional disciplines: the physical and biological sciences, engineering and mathematics. The product of research in these disciplines then becomes a part of the body of data on which applied technologies rest. In addition to this focus on disciplinary research, there is also an emphasis on innovative applications of new knowledge to energy problems, and on the early application and, if possible, direct commercialization of the results.

Some examples of BES research efforts impacting technology areas of major interest are: new research results on stress corrosion cracking that already are being used to evaluate intergranular corrosion of the nickel based alloys that are being used in nuclear steam generators; several projects related to nuclear waste isolation which have provided new insights into important aspects of plutonium migration: these include effects of chemically active leachants generated in the focal aqueous medium by the high radiation field itself, immobilization effects of soils rich in organic humic materials, and the radiation stability of a simulated mineral planned to be a component in a long term storage host material for nuclear waste.

A solar related research result has been the experimental observance of a phenomenon in light-excited semiconductors which could lead to a doubling in the efficiency of photo-electrochemical solar devices. Related to transportation, conservation or electric generation technologies, the scientific feasibility was the demonstration with BES support of producing batteries, both storage and primary, with electrodes made of light-weight polyacetylene sheets. The successful demonstration of this concept can pave the way for a whole new technology and considerably improve the outlook for electrically powered vehicles.

The Energy Research Analysis (ERA) program provides the capability for independent, rigorous assessment of the base of research that underlies a variety of energy technologies. Assessments are consolidated under one organization, the Office of Energy Research, in fulfillment of legislated responsibility for the Director to advise the Secretary on the agency's research and development programs.

The University Research Support (URS) program consists of two major subprograms and a set of program activities focused on the following three primary objectives: To strengthen university capability to do energy research; to strengthen the quality and increase the number of students interested in pursuing energy-related professional careers; and to enhance technology transfer activities through cooperative research efforts between universities, the agency's national laboratories and private industry. The first subprogram, University/National Laboratory Cooperative Research, is directed at strengthening the capabilities of both universities and national laboratories as major energy research performers in the conduct of long range energy research. Many of the activities supported within this subprogram involve joint efforts between university and laboratory-based researchers. The second subprogram, Energy Manpower Development, includes efforts to increase the number of students pursuing energy-related engineering and science careers. This subprogram also includes the Department's statutory responsibility for assessing the supply and demand of manpower for both current and projected energy R&D programs.

The University Research Instrumentation (URI) program supports the purchase by the major research universities of state-of-the-art, scientific instrumentation used in energy-related research areas such as combustion, biological energy conversion, catalysis, radioactive waste management and engineering research.

The goal of the Multiprogram General Purpose Facilities (MGPF) program is to provide for the rehabilitation and replacement of general support facilities which are essential to the continued operations of the agency's multiprogram laboratories. Multiprogram General Purpose Facilities are facilities which are suited to many different users and programs; these are roads, railroads, site utilities, and support buildings such as laboratories, office buildings, shops, warehouses, etc. They are restricted to facilities where no one program uses more than approximately 60 percent of the facility.

The replacement cost of the existing general purpose facilities at the multiprogram laboratories exceeds $6,500,000. The MGPF program is required to maintain this investment and to ensure its viability. The program will be required as long as the multiprogram laboratory facilities are utilized to perform research and development functions for the agency. The program is an appropriate Federal role reflecting the responsible management of the Government's real property. The program is based on the premise that through continuous usage and aging, facilities deteriorate over time to a point where they are no longer useful to perform their intended functions and must be rehabilitated or replaced.

Advisory and Oversight Program Direction provides funds for the personnel resources required by the Director of Energy Research to carry out his responsibilities specifically assigned by legislation (P.L. 95-91) as well as those mandated by the Secretary in areas beyond the scope of the Energy Research and development program in order to advise the Secretary with respect to the well-being and management of the multiprogram laboratories; supervising or supporting research activities carried out by any of the Assistant Secretaries; and providing for program management of the Energy Research Analysis, University Research Support, and Multiprogram General Purpose Facilities programs. The program provides funds only for the salaries and related personnel expenses for the personnel who carry out the studies, analyses, monitoring and coordination activities required to support the Director. It does not include any funds for outside contracts.

The Office of Energy Research Policy and Management program provides for the salaries and related expenses associated with staff in the immediate office of the Director, Office of Energy Research, and in the Office of Management.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
LEAD TABLE
BASIC ENERGY SCIENCES
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
(Tabular dollars in thousands. Narrative material in whole dollars.)

	1983 Appropriation	1984 Appropriation	1985 Base	1985 Request
Basic Energy Sciences				
Materials Sciences				
Operating Expenses	$108,163	$125,110	$125,110	$141,480
Capital Equipment	8,510	12,780	12,780	15,450
Construction	3,000	16,440	16,440	31,720
Subtotal	119,673	154,330	154,330	188,650
Chemical Sciences				
Operating Expenses	70,000	75,500	75,500	80,930
Capital Equipment	5,510	6,520	6,520	8,840
Construction	400	450	450	8,050
Subtotal	75,910	82,470	82,470	97,820
Nuclear Sciences				
Operating Expenses	30,644	37,900	37,900	49,755
Capital Equipment	1,556	2,150	2,150	2,950
Construction	0	270	270	300
Subtotal	32,200	40,320	40,320	53,005
Applied Mathematical Sciences				
Operating Expenses	13,850	14,670	14,670	28,250
Capital Equipment	800	970	970	1,500
Subtotal	14,650	15,640	15,640	29,750
Engineering and Geosciences				
Operating Expenses	17,200	19,000	19,000	20,795
Capital Equipment	1,120	1,150	1,150	1,500
Subtotal	18,320	20,150	20,150	22,295
Advanced Energy Projects				
Operating Expenses	8,300	9,100	9,100	10,810
Capital Equipment	290	310	310	320
Subtotal	8,590	9,410	9,410	11,130
Biological Energy Research				
Operating Expenses	9,500	10,580	10,580	12,490
Capital Equipment	370	400	400	560
Subtotal	9,870	10,980	10,980	13,050
Program Direction				
Operating Expenses	3,170[a/]	3,970	3,970	3,830
Subtotal	3,170	3,970	3,970	3,830
Total				
Operating Expenses	260,827[a/]	295,830	295,830	348,340[b/]
Capital Equipment	18,156	24,280	24,280	31,120
Construction	3,400	17,160	17,160	40,070
Basic Energy Sciences	$282,383[a/]	$337,270	$337,270	$419,530[b/]
Staffing				
Total FTE's	56	62	62	62

Authorization: Section 209, P.L. 95-91

a/ Funding level above reflects a comparability adjustment of $70,000 and 1 FTE in connection with the Applied Mathematical Sciences subprogram.

b/ This decision unit reflects $3,000,000 for savings resulting from management initiatives in the area of administrative processes/field structure.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
SUMMARY OF CHANGES
BASIC ENERGY SCIENCES
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
(thousands of dollars)

1984 Appropriation enacted	$337,270
Operating Changes	
Programmatic increases (described in detail below)	
Materials Sciences	+16,370
o Provides for increased funds for facility operations, reactor fuel element requirements and additional requirements associated with the advanced materials research initiative	
Chemical Sciences	+ 5,430
o Provides increases for meeting facility commitments and reflects internal adjustments required to meet ongoing research commitments.	
Nuclear Sciences	+11,855
o Provides increases to meet commitments for the National Nuclear Data Program, an expansion to the Heavy Ion Fusion Program, and to meet facility commitments.	
Applied Mathematical Sciences	+13,580
o Provides increases for a significant expansion in basic research in scientific computing at national laboratories, universities and private research institutions. In addition, experimental computing capabilities are being established to support the exploration of new concepts in large scale scientific computing. Also, increase is provided for expanding access to Energy Research scientists to state-of-the-art computing capability.	
Engineering and Geosciences	+ 1,795
o Increases are provided to expand the number of scientists and engineers in these areas of research.	
Advanced Energy Projects	+ 1,710
o Increases permit an expansion to the number of research projects supported by this subprogram.	
Biological Energy Research	+ 1,910
o Increase will begin to address plant and microbial sciences research for interdisciplinary research groupings to focus on specific problems.	
Program Direction	- 140
o Reflects lower administrative support costs.	
Subtotal Operating Changes	52,510

Capital Equipment Changes

o Programmatic increase in each of the subprograms will be provided to meet facility requirements, to support the recently assigned responsibility for General Purpose Equipment at Argonne National Laboratory, and to support new requirements in areas of increasing research	+ 6,840
Subtotal Capital Equipment Changes	6,840

Construction Changes

o Programmatic increases for General Plant Projects (Argonne National Laboratory, Ames Laboratory, Notre Dame University, and Stanford University); Accelerator Improvement Projects; Kansas State University Ion Collision Physics Facility; National Synchrotron Light Source; Center for Advanced Materials and Stanford Synchrotron Radiation Laboratory Enhancement	+22,910
Subtotal Construction Changes	22,910
1985 budget request	$419,530

Overview

The FY 1985 request for the BES program is $419,530,000. Reflected in this budget request is $3,000,000 in savings from management initiatives in the area of administrative processes/field structure. This budget which is composed of $348,340,000 in operating funds, $31,120,000 in equipment funds, and $40,070,000 in construction funds, maintains the needed continuity of the FY 1984 program. An increase needed for facility operations and research will be provided; the principal goals of the research program and the goals of the new initiative in materials sciences will be met, the first step in expanding Energy Research computing activities to meet immediate needs for supercomputer access by ER researchers will be taken, and enhancements will be permitted in the most promising, selected areas of research.

In determining the appropriate Federal roles in the support of RD&D, the Administration has identified the support of long range basic research as the particular responsibility of government and, further, that "mission agencies should support the foundation of basic science, as well as mission-oriented applied research, in appropriate disciplines." The Basic Energy Sciences (BES) program is responsible for generic long-range energy related research in the Department of Energy (DOE). The research supported by this program has as its principal focus energy, but also supports a number of other important national goals. Because of the ramifications of technical breakthroughs, it is fair to say that national security, U.S. leadership in science and technology and training are all equally served by an aggressive program in basic research.

Improvements in existing technologies and the development of new technologies invariably come from the application of new scientific knowledge. External blue ribbon advisory groups have repeatedly recommended that DOE increase its funding of basic research and have called for BES to be given a larger role in developing the needed research base for the different energy supply and conservation options. BES has endeavored to respond to these recommendations. In FY 1984 a major new materials initiative was proposed that not only attempts to deal with advanced materials research but also with aspects of training new researchers. This initiative which will continue in FY 1985, and will result in the redirection of a major DOE laboratory, the Lawrence Berkeley Laboratory, which was recommended in a recent report of DOE's Energy Research Advisory Board.

The major product of the BES program is knowledge relevant to energy exploration, production, conversion and use; that product becomes a part of the body of information on which the applied technologies rest. While the pursuit of research by BES to broaden the technology base needed for identified energy technology options is extremely important, perhaps even more important is the need for basic research unfettered by preconceived notions of what technologies will be important several decades from now, so that new, currently unidentified options may emerge.

In support of basic research activities, BES supports a number of national user facilities. Recently four such facilities have been brought on line and each promises to open whole new areas of research possibilities heretofore not possible. These new facilities are: the National Synchrotron Light Source at BNL, the Intense Pulsed Neutron Source at ANL, and the 1.5 Mev high voltage electron microscope at LBL, for all of which FY 1983 has been the first full year of operation, and the Atomic Resolution Microscope at LBL, where the first full year of operation will be FY 1984. BES also undertook the responsibility for the operation of the Stanford Synchrotron Radiation Laboratory (SSRL), our second major research facility for synchrotron radiation. The coming of age of these new major facilities together with existing ones is placing an added burden on BES to provide the additional funding needed for their operation at levels commensurate with the needs of the researchers. BES also is undertaking provision of access to supercomputers to ER researchers through the Applied Mathematical Sciences subprogram.

Examples of research progress by the BES subprograms and their relationship to long term energy problems offer an insight into the nature of the BES program.

In the Materials Sciences subprogram the research is directed towards understanding basic materials phenomena and classes of materials important to energy systems. This past year it was found that, in metals, helium itself forms lattice defects which nucleate gas bubbles. This discovery alters present thinking on the role radiation damage plays in helium bubble formation in metals, a new insight that needs to be explored more deeply for fission and fusion systems where helium is generated by nuclear reactions. A second accomplishment in this subprogram has been the preparation of simple, yet highly efficient solar cells by glow discharge implantation doping of single crystal silicon followed by pulsed laser annealing; this process is expected to be commercially feasible.

Under the Chemical Sciences subprogram, it was found that the phase behavior for fluids under shear is different from fluids "at rest" and depends on the strain rate; this helps explain observations of anomalous phase separations under flow conditions and enhances our capabilities for predicting thermophysical properties of complex fluids and for modeling reaction systems. There have been several advances involving photochemistry: one has been the photocatalytic splitting of water to produce hydrogen using visible light and inexpensive modified iron oxide photoelectrodes; a second has been the discovery, with use of a newly devised light saturation technique, of the existence of one or more previously unsuspected chemical sequences in the chloroplast-ferrodoxin-hydrogenase photosynthetic system, a discovery which adds importantly to the arsenal of knowledge available for attempting practical water splitting technologies.

Under the Nuclear Sciences subprogram, the nuclear data measurements activity has been concentrating efforts on the neutron and gamma ray emission induced by fast neutrons on materials of interest to the fusion program. A new high resolultion gamma ray detector system to further theoretical understanding of inelastic neutron scattering phenomena has become operational.

Within the Engineering and Geosciences subprogram, basic studies of the effects of fluids in pores or sound waves transmission in rocks has led to discovery of a new approach to monitoring recovery of heavy oils. A field test of the new method is being sponsored by the oil industry.

The Applied Mathematical Sciences subprogram has demonstrated significant progress in the design of new fast algorithms for parallel machine architectures for several classes of computational models used in combustion experiments, reactor safety, plasma physics and weapons design. Five new parallel processor systems reached the engineering prototype stage and are successfully running problems at universities and laboratories.

A recent accomplishment under Advanced Energy Projects has been the measurement, for the first time, of fusion reaction rates in a scheme utilizing mu mesons as reaction catalysts. The reaction yield of neutrons is high and potential application of the concept to provide high intensity neutron sources is possible. The examination of such novel concepts is a unique feature of this subprogram.

The Biological Energy Research subprogram has made progress on a subject of major importance in the burgeoning field of genetic engineering. The successful use of Agrobacterium Ti plasmid, a DNA vector found in a bacterium that is particularly useful to introduce "alien genes" into higher plants has been marred by an unwanted side effect, tumor formation in the recipient plant. The significant accomplishment under this subprogram has been the actual elimination of the one gene responsible for tumor formation.

BES considers the merits of research in relation to the diverse needs for energy and selects those topics that, when taken as a whole, comprise an optimum, balanced program of mission-oriented basic research. To carry out this program, BES plans, supports and administers energy related research in the physical, biological and engineering sciences. New scientific information in these areas addresses the Administration's goals by providing the fundamental scientific and engineering base on which the Nation's future energy options depend. The strategy continues to be to:

- o Provide critical knowledge and data and develop trained scientific talent through support of highly competent scientists in DOE mission areas;
- o Provide for, and support operation of unique, specialized research facilities;
- o Maintain liaison with other DOE programs, federal agencies and the scientific, academic and industrial communities;
- o Seek the scientific and industrial communities' assistance for the identification of needs and opportunities for research in areas likely to be relevant to future energy options; and
- o Promote early applications of the results of basic research.

To continue its effectiveness, the Basic Energy Sciences program must: 1) maintain a strong core program -- this involves equipping, supporting and encouraging the scientists involved in our current program activities, and the training of new, younger scientists, to expand the forefront of knowledge in areas likely to be important to future energy technologies; and 2) continue to support existing, unique facilities important to research in the U.S. while at the same time providing for needed new facilities and for their operation; and 3) create opportunities for exploiting new, emerging areas that have been identified as having great potential importance to energy.

Prime examples of needed new facilities and opportunities for growth are contained in the Advanced Materials initiative which was proposed as part of the FY 1984 budget and continues in FY 1985. The Center for Advanced Materials portion of the initiative will serve as a logical redirection of one of the Department's major national laboratories and will accomplish these important objectives:

1. Establishment of a basic research program strongly oriented toward the solution of technologically important problems with major industrial input and research participation. Heavy emphasis will be placed on the synthesis, characterization, and study of the properties of advanced materials.

2. Provide advanced facilities for research training of additional graduate students in physical sciences and engineering fields vital to U.S. high-technology industry.

	FY 1983	FY 1984	FY 1985 Request
Materials Sciences			
Operating Expenses	$108,163	$125,110	$141,480
Capital Equipment	8,510	12,780	15,450
Construction	3,000	16,440	31,720
Subtotal	119,673	$154,330	$188,650

The goal of the Materials Sciences subprogram is to increase our understanding of phenomena and properties important to materials behavior which will contribute to meeting the needs of present and future energy technologies. This program is important because it underpins the high technology industrial areas of the Nation, pushes forward the frontiers of knowledge in this fundamental technical area, and trains new scientists in this highly interactive field, in addition to working on the long range problems of energy systems. It is well known that materials problems and limitations often restrict the performance of current energy systems and the development of future systems. A few examples of such problems and limitations include: low conversion efficiency in photovoltaic materials, radiation damage in fusion systems, thermal and mechanical stability of materials for heat engines, and corrosion and erosion of critical components in coal conversion plants. The Energy Research Advisory Board had placed the highest relative program ranking on this area of research in a review of major energy science and technology base programs last year and is currently undertaking an in depth study of all materials research and development in the Department.

While each Federal agency conducts materials research to meet its own particular objectives, coordination across agencies is readily accomplished through established committees and interactions. In the area of basic materials research, the Materials Sciences subprogram is most interactive with the National Science Foundation's Materials Research Division and the more basic programs of the Department of Defense. The unique aspect of the Materials Sciences subprogram is the focus on energy related research and the use of advanced diagnostic techniques made possible by state-of-the-art research facilities supported by this subprogram. These activities complement the NSF and other agency programs. The research is needed to carry out the mission of the DOE. It is different in both character and its interactions with other programs. Although the NSF program has significant breadth, it does not have the concentration in energy systems materials research. For example, there is relatively little work in the NSF program on radiation effects, corrosion-erosion related to fossil energy systems, solar photovoltaic materials, or nuclear waste isolation materials, whereas the Materials Sciences subprogram has very significant efforts in these areas. This subprogram also has large efforts in facility-related research such as neutron scattering, synchrotron radiation research and electron microscopy, compared to the relatively small efforts in the NSF program. The Materials Sciences subprogram has traditionally provided the development, construction and operation of large facilities for the total national program. Use of these major facilities is now formally open to all qualified researchers. A recent survey of twelve of the collaborative research centers under the purview of the Materials Sciences subprogram has shown that they accommodated about 900 users during the past year. The users came from DOE laboratories (21 percent), universities (48 percent), industry (14 percent), and the remainder from other organizations. The replacement cost for these facilities is estimated at $450,000,000. The Materials Sciences research funding around these facilities in FY 1983 was about $16,000,000 with another $11,000,000 being attracted from outside the Materials Sciences subprogram.

As in FY 1984, and in response to Congressional interest in materials research and in consonance with the President's materials policy statement, an Advanced Materials Research initiative is being continued. This initiative is described separately and builds upon the base of knowledge established by the Materials Sciences program and other such programs in the Government. It will complement ongoing core program activities, and emphasize high risk, high pay-off research with potential for technology transfer.

The FY 1985 request includes the following amounts for the Core Program: $132,110,000 for operating, $13,300,000 for capital equipment and $1,800,000 for construction. For continuation of the initiative on Advanced Materials Research, $9,370,000 is included for operating, $2,150,000 for capital equipment, and $29,920,000 for construction.

The field of materials sciences is timely for exploitation as a result of many new advances. We are approaching the ultimate resolution in microscopy. The LBL Atomic Resolution microscope has been installed and will begin research operation in FY 1984. Significantly enhanced spectroscopies are now available or will become available soon with new synchrotron radiation sources and neutron sources. The theory related to materials science is greatly improved although still difficult. Availability of high speed computers will help this area. Coupling these experimental and theoretical advances with our improved ability to prepare new materials will open up opportunities to design materials from fundamental principles and overcome or circumvent known and anticipated energy related materials problems. A recent National Academy of Sciences report on Materials Science supports this same general conclusion.

Some of the needs to which the Materials Sciences research ultimately contributes include:

- Developing new or substitute materials
- Tailoring materials to satisfy defined requirements
- Predicting materials problems and service life

- Improving the ability to successfully attack unforeseen materials problems in advanced energy systems, and

- Improving the theoretical and experimental capability to analyze the fundamental structure of materials

To provide the new knowledge and information to meet these needs, Materials Sciences, comprised of the subfields of metallurgy, ceramics, solid state physics, and materials chemistry, places emphasis on selected generic areas of fundamental importance and on areas where problems are known to exist or are anticipated. Some research is directed at a single energy technology (e.g., photovoltaic materials for solar energy conversion), some research would have applicability to many technologies simultaneously (e.g., embrittlement of structural materials due to the presence of hydrogen), and still other research has more fundamental implications underpinning all materials research (e.g., mechanisms of atomic transport of solids). The research is conducted among a variety of institutions--national laboratories, universities, and to a lesser extent, industry utilizing the talents of metallurgists, ceramists, solid state physicists, and materials chemists.

In addition to maintaining an appropriate mix among long-term science, multi-technology and single energy technology oriented research, a balance must be retained between forefront large facility-related research and small individual projects. Certain types of research simply cannot be carried out without large facilities (e.g., neutron sources with significant fluxes of neutrons cannot be made in "small" sizes). Also newer instruments with significant improvement in capability (e.g., synchrotron radiation sources) are very expensive to build and operate. The Materials Sciences subprogram utilizes several major facilities in the pursuit of its research goals, including the National Synchrotron Light Source (NSLS) BNL, High Flux Beam Reactor (HFBR) BNL, High Flux Isotope Reactor (HFIR) ORNL, Intense Pulsed Neutron Source (IPNS) ANL, Ion Implantation Facility ORNL, and Electron Microscopes at ORNL, ANL, LBL and the University of Illinois. Operation of facilities in FY 1983 required about 20 percent (and is increasing) of the operating budget of the Materials Sciences subprogram, not including the unique research associated with them. These facilities also are available to qualified users outside the national laboratory complex.

Current emphases and trends in the core program indicate utilization of the major user facilities will increase. The university portion of the program will be maintained at about 20 percent. When including Ames Laboratory (Iowa State University) and Lawrence Berkeley Laboratory (University of California) the support going to universities is approximately 38 percent. Research will be strengthened in the areas of organic-polymer conducting materials, surface modification utilizing ion implantation and laser or electron beam treatment, structural ceramics, condensed matter theory, critical materials substitution, and materials preparation among others.

This subprogram supports both directly and indirectly the development of a national position on critical materials, welding and rapidly solidified materials. The ability to provide such support stems directly from the experience and continuity within the Materials Sciences subprogram. The fundamental understanding of materials obtained in this subprogram has led to new approaches to alloy design for critical materials substitution, advances in welding and the science of rapidly solidified materials.

The subprogram utilizes workshops and reports of its Council on Materials Science (a non-Governmental body with representatives from academia, industry, and agency laboratories) to help focus on critical issues. Panel meetings on materials research at high pressure and materials aspects of nuclear waste isolation were conducted in 1982. During 1983, two panel meetings were held, one on surface modification and one on organic materials. The reports resulting from these workshops and panels are distributed widely, including publication in the open literature. Interactions and information transfer with the agency's applied materials research takes place through a

number of mechanisms including a formalized Research Assistance Task Force. Examples of these latter activities include meetings on fast ion conductors and corrosion related to batteries. Through these latter meetings the basic researchers learn of the problems in the applied programs and the technology oriented programs are exposed to scientists with a fundamental understanding of matter.

The Materials Sciences subprogram is the basic materials program in the agency underpinning all the energy technologies. Materials play a crucial role in the development of energy systems. Coordination among the agency's materials programs takes place primarily through the Energy Materials Coordinating Committee. Within the Federal Government, the subprogram is coordinated in part through the interagency Committee on Materials (COMAT) and the basic Interagency Materials Group. At the Federal program level, Materials Sciences continues to represent about one-third of the Federal Government support for basic materials research.

Materials Sciences is recognized throughout the research community for its excellence. Past technical accomplishments have moved into the technological or commercial sector (e.g., radiation resistant alloys, glassy metals, ion implantation techniques for surface modification, and superconducting wire), and it is expected that through the proven methods of technology/information transfer and effective management this year's accomplishments will likewise find use either for building our fundamental base of materials understanding or in some technological application in the future. It should be noted that industrial interactions with this subprogram are encouraged and indeed have been successful. Significant progress was made during the past year in many areas of the subprogram. Some examples of recent accomplishments include:

- o A new superconducting magnetic shielding method capable of sweeping out ambient magnetic fields to the nanoguass level has been demonstrated. This technique has the potential to revolutionize the methods of obtaining low and stable magnetic field environments necessary for low-noise operation of sensitive superconducting devices such as the Josephson Junction computer.

- o Simple yet very high efficient solar cells have been produced by glow discharge implantation doping of single crystal silicon followed by pulsed laser annealing. The method is easily automated and could radically change the manufacture of solar cells.

- o A new method was developed for the homogeneous addition of sintering additives to silicon nitride, and a procedure was derived to prevent the agglomeration of colloidal-sized powder. Homogenity and retention of colloidal particle sizes are essential requirements in order to sinter silicon nitride to obtain reliable components for ceramic engines.

- o A study of simulated radioactive waste glass forms using uranium to substitute for transuranic elements has shown that they do not provide a reliable simulation of the structure and bonding properties of transuranics in silicate glasses. Since the leaching properties are dependent on bonding, this result indicates real waste systems must be investigated for reliable prediction.

- o Neutron "time-of-flight" techniques have been used to successfully measure residual stresses in tungsten carbide cermet materials and in a zirconium alloy. The information on cermet materials is important in the design and development of drilling inserts for oil and gas well drilling apparatus. The detailed information on residual stresses in the zirconium alloy provides valuable data for reactor fuel element and pressure tube design and performance analysis.

- o It has been demonstrated that the structure and surface hardness of ceramic surfaces can be modified and controlled by means of ion implantation. The properties that were obtained could be further changed by means of post-implantation thermal annealing.

- o An effective method was developed which accurately describes the strain field around a crack in a class of materials termed "incompressible-fully plastic," known to be the most relevant to heavy section piping and pressure vessels in energy plants.

- o It was predicted and discovered non-energetic helium forms lattice defects in metals to nucleate gas bubbles. This understanding alters present thinking on the role displacement producing radiation damage plays in helium bubble formation in metals and this must be regarded as a potential problem area in fission and fusion systems.

The request for the Materials Sciences core program will provide for needed continuity and permit a reasonable level of utilization of major facilities, strengthening of important topical areas and initiation of some new thrust areas recommended by workshops and panels of the Council on Materials Science. Of the $14,700,000 increase in operating funds in the core program over FY 1984, the most significant amount is for facility operations ($6,500,000) including increased costs for reactor fuel elements, and research ($2,700,000) at newer major facilities. The operational funding for NSLS will increase, which together with the Chemical Sciences funding for NSLS will allow NSLS to run about 19 out of a maximum of 21 shifts per week. Additional funding will be allocated to the other major facilities for operational costs, for example to the LBL Center for Electron Microscopy in order to permit close-to-optimum outside use.

The increase in equipment funds will permit the completion of the surface modification laboratory at ORNL ($500,000) and the analytical electron microscope at ANL ($950,000). The increase will also allow purchase of equipment for the low temperature neutron irradiation facility ($200,000), neutron scattering equipment ($800,000), synchrotron radiation equipment ($300,000), and electron microscopy equipment ($200,000). Accelerator and Reactor Improvement funds are requested for NSLS ($1,100,000), HFBR ($500,000), and the Bulk Shielding Reactor ($200,000) in the core program. Supporting information is provided in the construction project data sheet.

In addition to the Materials Sciences core program, continuing funds for the FY 1984 Advanced Materials Research initiative are requested. This was designed to satisfy a national need in materials science research, to undertake necessary forefront research outlined in various recent studies, and in response to Congressional interest and Administration policy. Funding for the second year, FY 1985, includes operating expenses ($9,370,000), capital equipment ($2,150,000), and construction ($29,920,000). United States economic health and national security requires the maintenance of a commanding lead in high technology and the reduction of vulnerability to critical and strategic imported materials. In response to this challenge, an Advanced Materials Research initiative was proposed in FY 1984. The FY 1984 initiative consisted of an expansion of activities at the National Synchrotron Light Source and the establishment on the West Coast of a new Center for Advanced Materials (CAM), which included enhancement of the Stanford Synchrotron Radiation Laboratory (SSRL). An ad hoc panel was established in April 1983 to review the proposed CAM. This request is consistent with the recommendations of that panel - to continue the initiative, but to delineate the synchrotron radiation sources from the materials research facilities and treat them separately. The panel made a number of constructive recommendations which are being used to shape the program and have been incorporated in this year's request. The Center for Advanced Materials will be organized to provide maximum benefit to the Nation. Industry will participate in the design and use of the facilities to assure that the research addresses America's high-technology needs. For example an advisory board composed of scientific leaders from industry, universities, and Federal laboratories will advise the LBL director on scientific program directions in CAM. An Industrial Fellows program will be established to provide joint LBL-industrial support for participation of outstanding industrial scientists in basic research studies of mutual interest to LBL and the scientists' parent companies. An initial workshop on industrial participation was held in 1983 where issues and follow on activities were agreed upon. A CAM Research Advisory Board has been established and workshops held for the initial research programs. Research teams from laboratories and universities will participate

in the design and development of advanced synchrotron radiation sources, and beam lines. In view of a new National Academy of Sciences study of major facilities for Materials Sciences, decisions to proceed with construction of major new facilities will await the results of that study.

This initiative includes funds for: A) three construction projects (Center for Advanced Materials-$10,790,000, Stanford Synchrotron Radiation Laboratory (SSRL) Enhancement-$9,130,000 and the expansion of capability at the National Synchrotron Light Source-$10,000,000); and B) research associated with construction and a forefront programmatic research program $12,550,000.

	FY 1985 Request
A. Construction	$ 29,920
1. Center for Advanced Materials	$10,790
2. Stanford Synchrotron Radiation Laboratory (SSRL) Enhancement	$ 9,130
3. National Synchrotron Light Source (NSLS)	$ 10,000

The Center for Advanced Materials project provides for the construction of two facilities at LBL: 1) a Surface Science and Catalysis Laboratory (SSCL); and 2) an Advanced Materials Laboratory (AML).

Surface Science and Catalysis Laboratory (SSCL)

The SSCL will further the fundamental understanding of surfaces of materials with a view toward applications and catalyzed processes on solid surfaces.

Advanced Materials Laboratory (AML)

The AML will create a forefront facility for the synthesis and characterization of materials of novel or optimized physical or chemical properties. In addition, it will provide a focus for development of innovative devices and use of advanced materials to assist in creating among other things possibly new types of heat engines. Innovative device concepts for more sophisticated characterization of materials properties or behavior will be developed.

Both SSCL and AML will build upon the very strong programs in materials science and in surface science and catalysis already in existence at LBL.

An enhancement program at the Stanford Synchrotron Radiation Laboratory (SSRL) will provide increased capability through the use of the PEP ring as a source of high energy (10-30 keV) photons, an advanced wiggler-based beam line for an unparalleled level of x-ray flux at SPEAR, and improved injection for greater time of use of SPEAR for synchrotron radiation. Provision will also be made for experimental set-up space to cut time losses for the many user scientists as they prepare to move experiments into place on SSRL's beam lines, and the laboratory and office spaces required to serve SSRL's much intensified pace of research use.

The third construction project will expand the capabilities at NSLS by allowing new beam lines to be built and by enlarging the existing building for the purpose of permitting additional experiments to be conducted. Construction of additional beam lines, including insertion devices, will be undertaken to accommodate the heavy use and demand by outside users from industry, universities, and other laboratories. The proposed building expansion will extend the northern perimeter of the existing building and add an additional floor above the existing office section.

Further details on each of these projects are provided in the construction project data sheets for Project 85-ER-111, 85-ER-112, and 85-ER-113.

	FY 1985 Request
B. Programmatic Research and Research and Development Associated with Construction.....	$ 12,550

Operating funds are needed for research and development to achieve the design goals of the construction projects proposed as part of this materials initiative. In particular, development is required in the advanced synchrotron radiation sources and the Stanford Synchrotron Radiation Laboratory (SSRL), and development funds are also needed for support of the National Synchrotron Light Source (NSLS).

At SSRL, development funds are needed for research on the PEP beam line undulator, the SPEAR beam line wiggler and for mirror and monochromator research. Operating funds are also included for SSRL, to begin the important Materials Sciences interaction with the research program there.

Related to the NSLS expansion, operating funds are requested to conduct research and development necessary for the construction of new beam lines. It is important to conduct research on advanced wiggler and undulators which will be inserted in x-ray and VUV rings. In addition, R&D will be performed on advanced mirrors and gratings for the x-ray microscopy and x-ray spectroscopy lines.

Research related to the Surface Science and Catalysis Laboratory (SSCL), will be undertaken to further the fundamental understanding of surfaces of materials with a view toward applications and catalyzed processes on solid surfaces. The FY 1985 effort will include programs on: atomic rearrangement of surface properties under extreme conditions and on new zeolites and novel catalyst characterization. A theoretical and experimental effort will be initiated in FY 1985 to use techniques already developed at LBL for characterizing atomic surface structures. Theoretical predictions will be based on the pseudopotential model and related approaches, which have been perfected at LBL recently, while experiments will be performed using advanced surface and photoelectron diffraction. The program will later become oriented toward materials of interest for new device concepts. Thus emphasis will shift from clean surfaces to overlayer systems (adsorbates, Schottky barriers) to atomic interfaces and three-dimensional structures. Surface structures will be altered with high-energy particles or intense photon fluxes which introduce line defects and point defects, and cause evaporation and phase transitions, including melting. Zeolites and other novel non-metallic catalysts will be synthesized and characterized using synchrotron radiation.

Programmatic research related to the Advanced Materials Laboratory (AML) will build on very strong ongoing programs in materials science at LBL. These programs, like others nationally, are handicapped by unavailability of novel and well-characterized materials for study. A particular objective of AML will be to create a forefront facility (for the synthesis and characterization of materials of novel or optimized physical or chemical properties); materials which may make possible devices, engines, or structures of superior performance in high technology and energy-related industries. Investigators in AML will collaborate with investigators in the Surface Science and Catalysis Laboratory (SSCL) by synthesizing and characterizing zeolites and novel new catalysts for investigation in SSCL. They also will collaborate with design engineers synthesizing new materials and materials improved properties. For example, initial research programs will focus on understanding the processing of polymers, the properties and behavior of new electronic materials including gallium-arsenide, and the processing of structural ceramics. In addition, research will utilize soft x-ray lithography to develop new experimental devices with dimensions of 100 Å or less. Success here would have an enormous effect on all electronic technology, perhaps most importantly on greatly advanced computers. The research will exploit exceptional properties of new materials in device concepts that have

the potential for dramatic improvements--orders of magnitude increases in limits of sensitivities of sensors, for example, and will investigate device concepts with potential for yielding order of magnitude improvements in characterizing material properties and behavior.

For FY 1985, the equipment needed includes the following: Survey and alignment apparatus for tolerances of a fraction of millimeter, equipment for ultra-high vacuum (UHV) for materials testing, RF development instrumentation in the two ranges 500 MHz and 2880 MHz, pulsed magnet equipment capable of 50 nanosecond rise times and low duty factor, low level electronics for beam monitoring, and control system equipment for hardware and software aids. Equipment for programmatic research includes advanced instrumentation for new material synthesis and characterization, e.g., a molecular beam epitaxy (MBE) system, ion-implantation and laser process instruments, and liquid phase epitaxial growth equipment. All of this instrumentation is for the advanced material synthesis in both solid and thin film form as well as for surface modification and coatings.

	FY 1983	FY 1984	FY 1985 Request
Chemical Sciences			
Operating Expenses	$ 70,000	$ 75,500	$ 80,930
Capital Equipment	5,510	6,520	8,840
Construction	400	450	8,050
Subtotal	75,910	82,470	97,820

The Chemical Sciences subprogram has two principal goals: to increase understanding of basic chemical and physical phenomena important to future energy production and conversion, and to promote the discovery of new concepts in chemical and physical aspects of energy processes. Within this framework the subprogram supports high quality research in a broad spectrum of chemical and physical scientific areas. Most of the research is conducted at national laboratories and universities, but research at not-for-profit institutions, other Federal laboratories and industrial laboratories is also supported.

Emphasis is placed on photochemistry, chemical physics, atomic physics, physical organic chemistry related to coal, catalysis, combustion thermodynamics of mixtures and separations. Continued research productivity in these areas is important, as is operation of two relatively new advanced major facilities and support of research efforts using them.

The Chemical Sciences subprogram provides the base support for operating the Sandia Laboratories' Combustion Research Facility, i.e., operating several state-of-the-art lasers, advancing their capabilities for users and providing services to visiting combustion researchers. Chemical Sciences is also the major source of support of basic research using this unique, world-class Facility. Its use by scientists from academia, industry and other laboratories is strong, both assisted by and in collaboration with in-house scientists. The facility has also been the center of limited exchange visits arranged through the International Energy Agency and through bilateral agreements with other countries entered into on a quid pro quo basis.

Chemical Sciences also provides about 40 percent of the support for operating the National Synchrotron Light Source (NSLS) at Brookhaven, and supports chemical sciences research using the NSLS. Following initial assembly and calibration, some initial experiments have been done on ionization of gaseous atoms by ultraviolet radiation. Other new areas of research have been initiated which are expected to help unravel questions in catalytic effects and combustion and to advance capabilities for analyzing the chemical elements in selected microscopic volumes at the surface of a solid. The areas of chemistry and physics emphasized in the Chemical Sciences subprogram are those most likely to produce advances in knowledge and understanding which will be valuable for improving energy technologies. In photochemistry, for example, progress is being made toward the understanding of photosynthesis, the sequence of processes by which nature utilizes solar energy to convert CO_2 to biomass.

Researchers in chemical physics are developing understanding and techniques for such diverse areas as catalysis and combustion. An example is extended x-ray absorption fine structure (EXAFS) research using synchrotron radiation, which is yielding information about the geometry and chemistry of adsorption and chemisorption of small molecules on the surfaces of catalysts. This will help explain and predict their catalyzed dissociation and rearrangement into larger fuel molecules.

Atomic physics researchers are attacking basic questions underlying the behavior of atomic and molecular ions, because of their importance to such areas as magnetic fusion, combustion, electric arcs and lighting.

Study of the fundamental chemistry of coal is adding new insights into the characteristics of different types of coal. It is likely that knowledge of the (sometimes subtle) differences among coals will allow future coal conversion plants to be designed for better control of product mixes or more efficient operations or both. The very basic research necessary to acquire this knowledge will be validated by careful steps being taken to assure reproducibility of results in coal experiments between different laboratories and over a very long time span (20 years or more).

Combustion, still the most important means of converting energy for years to come, is only partly understood. Chemical Sciences supports an outstanding assemblage of chemists and physicists who are using and enhancing state-of-the-art techniques to unravel the complex phenomena that make up combustion. Not only at the Combustion Research Facility but also at other laboratories, especially at universities, forefront chemical research is underway to help us understand the extremely fast sequences of chemical reactions that occur in combustion. Technological benefits can be looked for in combating pollution, gaining efficiency and tailoring combustion systems to future alternate fuels when petroleum and gas supplies dwindle.

Separations of fuels from wastes, more valuable fuels from less valuable fuels and desired chemicals from other chemicals always consume energy. Research in basic techniques of separations is therefore supported to widen the spectrum of methods from which designers of separative processes can choose the most efficient method for a given need. Related to this is a group of research projects in analysis, since almost all energy processes, especially separations, require devising of tailored analytical methods. Chemical Sciences' effort in analysis seeks general advances from which the specialized users can draw.

From the numerous achievements and contributions produced by Chemical Sciences researchers, those below are typical.

- A method for catalytic conversion of methanol (wood alcohol) selectively to ethanol (ordinary alcohol) has been discovered, using a homogeneous cobalt-based catalyst. This is an important advance toward using coal syngas for selective production of ethanol without forming the higher alcohols.

- A dual-possibility discovery: visible light may be either converted to electricity or caused to split hydrogen from water, by use of inexpensive thin film photocathodes of amorphous hydrogenated silicon. (The research was collaborative between a DOE-supported university and RCA.)

- A method has been discovered for estimating hydrogen atoms' transferability from donor solvents, which is important to evaluation of direct coal liquefaction processes. The method is based on relative kinetics of a free radical reaction involving the donor solvent and a diphenylazo compound.

- The first-ever measurements have been made of dielectronic recombination of multiply charged ions. This is an energy loss process in fusion type plasmas, which needs to be measured and understood. Colinear ion-electron beams were invented for this very difficult experiment.

- o A highly selective method has been discovered for determining ratios of isotopes in a sample, even for mixtures of isotopes of different elements but with the same mass number. It is based on laser-induced resonance ionization coupled with mass spectroscopy. The ability to make such measurements readily is important in advancing many areas of technology involving isotopes.

- o It has been discovered by techniques of molecular dynamics that the equation of state (phase behavior) for fluids under shear is different from fluids at "rest" and is dependent on the strain rate. Anomalous observations of phase separation under flow conditions are now understood and predictive techniques to estimate thermophysical properties of complex fluids now appear possible. (Work primarily funded by BES; some early support provided by NBS competence funds).

The request of $80,930,000, an increase of $5,430,000 for operating expenses, provides for maintaining the ongoing research. In addition, the recently constructed major facilities, NSLS and CRF, will receive support for their basic operations as they attempt to get up to speed in beneficial use of their advanced capabilities, in order to realize the most important national research advantages for which they were built. Their use by researchers in the areas of basic chemistry and physics noted above will promote scientific advances important to a wide scope of energy processes.

In the other parts of the Chemical Sciences subprogram cost-of-living increases will be given to photochemistry, atomic physics related to fusion, heterogeneous catalysis and supercritical properties of mixtures. Supported at close to the FY 1984 dollar level will be projects in radiation chemistry, molecular beam research, coal chemistry, analytical research and chemical engineering sciences.

In the paragraphs below which address the Chemical Sciences funding requests for capital equipment and construction, a new requirement appears which has a significant impact on the levels requested. For the first time, General Purpose Equipment (GPE) for the Argonne National Laboratory (ANL) and General Plant Projects (GPP) for ANL, the Ames Laboratory, the Notre Dame Radiation Laboratory and the Stanford Synchrotron Radiation Laboratory are included in the Chemical Sciences budget request. These will be detailed below. Taken together, they add $7,750,000 to the requests. They have previously been budgeted in the Breeder program and in other parts of the BES program. The major share of this shift is specifically associated with the assuming by BES of landlord responsibility for ANL beginning in FY 1985. A significant backlog has developed at ANL for both GPE and GPP items. The capabilities of the Laboratory have been jeopardized as a result. The FY 1985 budget attempts a first step in a necessary replenishment in these two areas.

The FY 1985 budget request of $8,840,000 for capital equipment includes, for the first time, $2,000,000 for GPE at ANL, as mentioned earlier. It also includes $140,000 for GPE at the Ames Laboratory. The remaining $6,700,000 in the request is $320,000 above the level contained in the FY 1984 budget. It represents a continued attempt to replace equipment researchers are using. At the same time other requirements must be served: replacement of outworn equipment, the equipping of the Chemical Sciences part of the National Synchrotron Light Source and continued rounding out and advancement of the largely laser based equipment at the Combustion Research Facility.

The FY 1985 request for construction, again an explained above, includes for the first time, GPP funding at ANL ($5,000,000), the Ames Laboratory ($600,000), Notre Dame Radiation Laboratory ($50,000) and the Stanford Synchrotron Radiation Laboratory ($100,000).

For the Chemical Sciences subprogram itself, a significant construction project is requested for the Kansas State University Ion Collision Physics Facility and associated machines. In FY 1985, $2,000,000 is requested for this project which has a total cost to the Federal Government of $3,400,000. This facility will combine a remarkably high current source of highly charged, low velocity ions with existing accelerator-based research capabilities. The combination will be known as the Atomic Collision Physics

Institute; the State of Kansas will provide added funds for the building portion of this project. With the addition of this facility, US competitiveness in accelerator-based atomic physics, important for both basic scientific advances and fusion technologies, will be restored.

Finally construction funds for two Accelerator and Reactor Improvement and Modification projects are requested. At Argonne $200,000 will go to modification of the ANL ATLAS' accelerator to incorporate a beam line for atomic physics research. This will make available a high velocity beam of multiply charged heavy ions for study of interactions with atoms, ions, molecules, electrons and photons. The resulting knowledge will impact magnetic fusion and other energy technologies. At Brookhaven, $100,000 will allow improvements to be made to the x-ray facility at NSLS in order to permit atomic physics research. The improvement will enable research to be done on the interactions of intense, high energy x-rays with atoms and ions.

	FY 1983	FY 1984	FY 1985 Request
Nuclear Sciences			
Operating Expenses	$ 30,644	$ 37,900	$ 49,755
Capital Equipment	1,556	2,150	2,950
Construction	0	270	300
Subtotal	32,200	40,320	53,005

Objectives of the Nuclear Sciences subprogram are: (1) measurement, compilation, and evaluation of nuclear data for fission and fusion energy technologies; (2) improvement of our knowledge of the chemical and physical properties of the actinide elements; (3) assurance of the availability for research of both isotopically enriched samples of the ordinary elements and samples of the man-made transplutonium elements; (4) operation of the Stanford Synchrotron Radiation Laboratory (SSRL), which shares use of the Stanford Positron Electron Asymmetric Ring (SPEAR) with the High Energy Physics program (Responsibility for operation of the SSRL was transferred from the National Science Foundation to BES in FY 1983); and (5) research on heavy ion accelerator technology and preparation for its evaluation as a driver for inertial confinement fusion applications.

The FY 1985 request includes $49,755,000 for operating expenses and $2,950,000 for capital equipment. Each of these activities which comprise this subprogram is discussed further below.

Nuclear Data

The goal of the Nuclear Data activity is to establish and maintain an accurate, complete, and accessible nuclear data base to meet long-term needs of the fission and fusion energy technologies and to support nuclear waste management and weapons development activities of the Department. The United States nuclear data effort is a well-integrated, time-tested activity involving data measurement, compilation, evaluation, processing, and dissemination. Measurement work is centered at the Oak Ridge Electron Linear Accelerator (ORELA); the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory is the focus of compilation and evaluation efforts.

Beginning in FY 1985, the Nuclear Science subprogram will assume greater responsibility for management and support of the national nuclear data system. In coordination with this subprogram, other nuclear-based programs (Nuclear Energy, Fusion Energy, Nuclear Regulatory Commission, and Defense Programs) are expected to participate by supporting data activities unique to the particular requirements of their respective technologies. This Nuclear Data activity will assume responsibility for the overall quality and breadth of the national nuclear data effort. The light water reactor industry participates in Cross Section Evaluation Working Group (CSEWG) activities and provides funds for special data projects through the Electric Power Research Institute (EPRI).

The request for FY 1985 ($11,380,000 operating and $700,000 capital equipment) maintains the overall DOE nuclear data activities at levels matched to national needs. This BES request includes funding for essential elements of the national nuclear data system that have previously been supported by Nuclear Energy. These elements include selected activities at Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Idaho National Engineering Laboratory (INEL), and Oak Ridge National Laboratory (ORNL).

Nuclear data needs are documented in great detail and are regularly updated: for the fission technology, as a part of the duties of the CSEWG; for the fusion technology, as a part of the duties of a special working group of the United States Nuclear Data Committee. The Office of Fusion Energy provides direct input to this special working group.

An important evaluation effort is currently under way involving scientists from the National Bureau of Standards (NBS), Los Alamos National Laboratory (LANL), ORNL and BNL who are attempting for the first time a simultaneous best fit to the major standard cross sections used in the Evaluated Nuclear Data File (ENDF), incorporating all the information on the covariances or correlations of the data measurements. Work is also proceeding on extensions of the ENDF formats that will permit the inclusion of more detailed data and make the file more useful for applications involving higher energy neutron reactions, e.g., fusion technology.

The second data base activity, the Evaluated Nuclear Structure Data File (ENSDF), is supported entirely by BES (with the exception of non-U.S. participants) and consists of a network of evaluators of "mass-chains" in the United States and abroad. Coordination, assembly, and production of the data file and the important continuing publication of revised "Nuclear Data Sheets" is performed by the NNDC. The United States ENSDF evaluation effort includes contributions from BNL, INEL, Lawrence Berkeley Laboratory (LBL), ORNL, and the University of Pennsylvania. A Radioactivity Handbook based on ENSDF is being prepared at LBL.

The BES Nuclear Data activity also includes a Nuclear Data Measurement effort in which the talents of experienced nuclear physicists are used at appropriate facilities to perform the difficult, painstaking measurements required to improve the data base. The major effort is carried out at the Oak Ridge Electron Linear Accelerator (ORELA). There, neutron cross sections can be measured efficiently with great resolution and over a wide range of energies. Three small university groups collaborate with ORNL staff in experimental work at the ORELA.

Measurements under way at the ORELA include studies of fast neutrons on materials of interest to the Office of Fusion Energy. A new high-resolution gamma-ray detector system has been developed for use in experiments designed to improve the understanding of neutron inelastic scattering at the higher energies of interest to the Fusion Energy program. Detector systems are being designed and tested to determine the capability of the ORELA to measure neutron-induced charged-particle spectra over a wide range of neutron energies and angles. For the fission technology, precise total cross section measurements from 0.01 eV to about 10 eV neutron energy will be carried out at the ORELA to determine resonance parameters of important fuel nuclides. The results should enable more reliable calculations of burn-up and a rational interpretation of applicable integral experiments.

Measurement efforts exploiting special facilities are carried out at several other national laboratories and at the NBS. Work devoted to the improvement of neutron standard cross sections is supported at the NBS, University of Michigan, University of New Mexico, and Idaho National Engineering Laboratory. Neutron cross-section measurements are also being supported at the University of Lowell, Ohio University, and the Triangle Universities Nuclear Laboratory (at Duke University).

Within the $500,000 in Capital Equipment funding requested for ORNL in FY 1985, $380,000 is planned for replacement of the 15-year-old computer used for data acquisition and on-line analysis at the ORELA with an efficient, modern computer system matched to ORELA's needs. To meet ongoing instrumentation requirements, a total of $200,000 is requested for BNL, INEL, LANL, NBS, and Pacific Northwest Laboratory (PNL).

Heavy Element Chemistry

This activity supports basic research in the chemical, physical, and nuclear properties of the actinide elements not only to increase our useful knowledge of these technologically important elements but also to contribute to a better understanding of the fundamental principles of physical science in general. Heavy Element Chemistry research supports a broadly-based effort in this area. The resulting knowledge meets some of the needs of DOE nuclear energy programs for specific information and data on the behavior of actinides in fuel reprocessing streams, in nuclear waste hosts, and in the environment. These high priority studies provide valuable information for the development and closure of the nuclear fuel cycle.

Research groups at national laboratories and universities are supported to pursue heavy element and radiochemical investigations. While some tracer work is done at universities, the study of actinide chemistry is largely limited to the national laboratories since high levels of radioactivity are involved. These laboratory facilities provide opportunities for visiting scientists from university and foreign labs to pursue collaborative research with the U.S. investigators.

A significant accomplishment of the past year was the first measurement of the metallic vapor pressure of the man-made element einsteinium. This is the heaviest and highest atomic number element for which this fundamental thermodynamic measurement has been made. The results confirm recent theories of the physical properties of the actinide metals and contribute significantly to our understanding of the actinide elements in particular and the relationship of these elements to the rest of the Periodic Table.

The recent National Academy of Sciences Workshop on the Future of Transplutonium Element Research recommended the maintaining and expanding of basic research in this field. Study of this region of matter of highest atomic mass is expected to provide new insights into the chemical, physical, electronic, magnetic, and solid state properties of matter in general.

Operating funds for Heavy Element Chemistry in FY 1985 are requested at the level of $5,125,000, an increase of $434,000 above FY 1984. These funds will maintain the ongoing program of the study of the actinide elements both for the increase of our fundamental knowledge as well as a better understanding for the solution of technological problems. Consideration will be given to specific recommendations of the Workshop and new experiments will be implemented.

The request for capital equipment is $350,000. This will provide for necessary replacements of some items of equipment and instrumentation used for the studies in the base program and for mounting certain of the experiments recommended by the Workshop.

Isotope Preparations

The electromagnetic isotope separation facility (Calutrons) at the Oak Ridge National Laboratory provides isotopically enriched materials for sale and loan [from a Research Materials Collection (RMC) or "loan pool"] to an international community for a wide variety of medical, industrial, and research applications. By far the majority of Calutron samples are stable (nonradioactive) isotopes. The DOE fission and fusion energy development technologies are critically dependent on a continuing supply of these materials for measurement of neutron reaction cross section data needed in reactor design and for an understanding of fission fuel behavior.

The isotopes of the heavy actinide elements are produced by sequential operations at ORNL's High Flux Isotope Reactor and the Transuranium Processing Plant (HFIR and TRU). The principal purpose of HFIR and TRU is to produce research quantities of the very high atomic number actinide elements for the use of the Heavy Element Chemistry and other DOE programs. These facilities are the sole source of californium-252 for the fabrication of neutron sources for loan and sale and for DOE research programs. It must be noted, too, that an important additional function of HFIR is providing one of the world's highest fluxes of neutrons. These are used by researchers in neutron scattering studies of solid state properties of matter and as a neutron irradiation source for the study of neutron damage of materials. Neutrons from HFIR are also used for the production of radioisotopes for research and sale. The costs for these research activities, other than providing the neutron flux itself, are not borne by the Nuclear Sciences budget.

The operating funds request for Isotope Preparations for the FY 1985 request is $16,970,000, an increase of $4,731,000 over FY 1984. Of this increase, $2,024,000 is needed for the higher cost of maintaining the operation of HFIR and TRU; another $1,020,000 is needed to expand Calutron operations to two segments for a full 12 months. This substantial increase is vitally needed to increase the production of stable and long-halflife actinide isotopes for DOE programs in research and technology development and for the buildup of depleted RMC inventories needed for research loans and for sales. Also in this increase, $1,450,000 more is needed to meet the projected HFIR fuel inventory increase and $237,000 is required to meet other programmatic requirements such as decontamination and decommissioning costs at the Mound Laboratory. Just as with the Materials Sciences support of the BNL High Flux Beam Reactor, this change in inventory costs stems from the higher cost of the newer fuel elements, the need to maintain an efficient level of effort in launching the new fabricator, and replenishing of the fuel inventory, which was drawn down during the change of fabricators.

The capital equipment request for Isotope Preparations is $650,000. Funds are requested to continue the Calutron modernization and upgrade program started in FY 1983. This facility was originally built during the Manhattan Project and most of the supporting equipment is seriously worn and unrepairable. New equipment is needed to minimize the possibility of component failure and facility shutdown.

In addition, $300,000 is requested for accelerator improvements at the High Flux Isotope Reactor. This project will provide for modifications to permit remote sampling of the containment atmosphere and the primary coolant. Emergency sampling components will consist of items such as the necessary piping, pumps, valves, instrumentation, penetrations, and collection stations. In the unlikely event of a fission product release to the primary coolant and/or the reactor containment system, the remote sampling capability would aid in evaluating the extent of the release and enhance the recovery process.

Stanford Synchrotron Radiation Laboratory

SSRL, a key facility in maintaining U.S. leadership in synchrotron radiation, provides high quality and steadily improving capabilities for much of the user community in the U.S. and the Free World. The radiation arises from either magnetically steering fast-moving electrons around the evacuated ring of the Stanford Positron-Electron Asymmetric Ring (SPEAR) or from sequences of magnets ("wigglers" or "undulators") inserted to affect the electrons' path. SSRL shares equally with the High Energy Physics program the operating time and costs of SPEAR. In the enhancing of SSRL's capabilities so as to help maintain the strong U.S. lead in synchrotron radiation research, SSRL works closely with LBL, other DOE laboratories and some leading industrial scientific organization such as Bell Laboratories, Exxon Research and Engineering and IBM. Coordination is also strong with other facilities such as the National Synchrotron Light Source. Research using this unique type of radiation is advancing rapidly especially because of these two major DOE facilities, opening new possibilities in understanding catalysts, physics of ions, crystal dynamics, biological functions on a molecular level, nonintrusive medical diagnostics to replace more hazardous procedures, and many more areas. The costs of supporting SSRL include a half share of operating SPEAR, for time periods dedicated to producing the desired energies and intensities of synchrotron radiation. SSRL costs

also include the staff and facilities to assist the visiting users with safety and operating procedures, since most of the users are scientists from other institutions (whose proposals have been carefully screened and reviewed by their peers). The FY 1985 request for operating funds for SSRL is $7,980,000, or $1,255,000 above the FY 1984 level. This increase is needed for several reasons: overdue correction of long standing understaffing; added people to assist with the growing number of experimental stations; increased efforts in development of SSRL's enhanced capabilities, some of these for DOE purposes; and strengthened research by SSRL's in-house scientists, at DOE's suggestion, in order to have sounder assistance to, and collaboration with, visiting scientists; and, finally, stepped up activities in preparing for use of the enhanced capabilities.

The requested FY 1985 capital equipment funds for SSRL are $600,000, a $110,000 increase above FY 1984. This is a tightly constrained equipment request in the above-noted framework of added activities.

Heavy Ion Fusion Accelerator Research

The goal of the Heavy Ion Fusion Accelerator Research (HIFAR) program is to develop heavy ion accelerator technology and perform appropriate ion-beam experiments to the point where an adequate data base exists for evaluation of heavy ion inertial fusion drivers and their possible use in civilian power applications of inertial confinement fusion.

The Heavy Ion Fusion Program was conducted by the Office of Inertial Fusion within Defense Programs from FY 1977 through FY 1983. In accordance with Congressional guidance and an agreement between the Assistant Secretary of Defense Programs and the Director of Energy Research, the accelerator research program was transferred to the Office of Energy Research. Beginning with FY 1984 funding has been sought directly for energy applications. Prior program accomplishments include numerous theoretical studies, conceptual designs, and minimal hardware studies. The promise of the heavy ion accelerator approach for fusion power has been the subject of a number of technical workshops and extensive reviews which have been uniformly favorable in their conclusions. A revised multi-year plan was formulated in connection with the transferred program. A recent JASON Panel considered the proposed National Plan for Heavy Ion Fusion to be a sensible next step in the program.

The revised program is based on the need for experimental verification of the previous theoretical studies at an appropriate scale. A two-stage plan has been formulated. The first stage (FY 1984-1986) primarily entails the research and development of critical elements of promising accelerator technologies with particular attention to the use of multiple beams for cost reduction. The second stage calls for a high-temperature experiment (HTE) in which a high temperature (50-100 eV) solid-density plasma would be created. Planned for FY 1987-1989, the HTE would entail the construction of an accelerator suitable for verification of the design principles of a reactor-driver accelerator and for verification that target heating predictions are correct. Production of high temperature in a solid-density plasma would represent a truly significant entry of accelerator technology into the parameter range needed for inertially confined fusion. It would settle questions relating to energy deposition and beam propagation, besides providing a crucial benchmark in the development of accelerators for fusion power. Given the long-established accelerator technology history that can guarantee repetition-rate, efficiency, and reliability, HIF could then be reliably evaluated as a serious candidate for a fusion power system for the next century.

In preparation for the high-temperature experiment it is crucial to have certain data from experimental tests on transport, acceleration, and the selected method for current amplification. Issues to be addressed in Stage I include: predicted transport space-charge limits on beam current; stability, reproducibility, and reliability of intra-pulse and pulse-to-pulse operation; accelerator cost reduction; preservation of beam quality including stability and containment of the high charge-density pulse; and final compression, transport, and focusing of the beam to the target.

The request for FY 1985 is $8,950,000 including $8,300,000 operating expenses and $650,000 capital equipment. This level of funds will provide 10 of an estimated 30 accelerating/focusing cells required for a "multiple beam experiment" which will serve to define and verify the HTE accelerator design. The remaining cells would be assembled in FY 1986. Principal FY 1985 milestones include completion of a multiple beam injector in addition to the 10 acceleration/focusing cells noted. The principal experimental work will be conducted at the Lawrence Berkeley Laboratory, with Los Alamos National Laboratory providing injector development and serving as lead laboratory.

Applied Mathematical Sciences	FY 1983	FY 1984	FY 1985 Request
Operating Expenses	$ 13,850	$ 14,670	$ 28,250
Capital Equipment	800	970	1,500
Subtotal	$ 14,650	$ 15,640	$ 29,750

The Applied Mathematical Sciences subprogram consists of two activities: Supercomputing Research and Energy Science Advanced Computation. The Supercomputing Research activity funds research in mathematical and computational sciences that is critical to the use and development of future supercomputer systems. The Energy Sciences Advanced Computation activity will provide network access to large-scale scientific computing required by several Departmental programs in the basic research activities funded by the Office of Energy Research in universities and national laboratories.

The first objective of the Applied Mathematical Sciences subprogram is to advance the understanding of the fundamental concepts of mathematics, statistics, and computer science underlying the complex mathematical models of the key physical processes in energy systems. Much of the scientific research and development effort throughout DOE programs is focused directly on analytical and numerical modeling of physical processes. An understanding of the fundamental principles upon which these models are based is important for developing energy systems for the future. Thus, research in mathematical analysis, algorithms, and computational techniques is crucial in conducting most scientific investigations.

The second objective is to meet the immediate needs for supercomputer access of the Department of Energy's High Energy and Nuclear Physics, Biological and Environmental Research, and Basic Energy Sciences programs and the long-range needs of the Department in computational research. This subprogram will make a substantial contribution to solving the national problems of providing access to supercomputers for energy researchers and ensuring that the U.S. maintains its lead in computational sciences related to supercomputer technology.

Supercomputers are playing an increasingly important role in many of the Department of Energy's programs. Every generation of large scientific computers has had a significant impact on the ability of the DOE laboratories to meet their mission goals. Each new machine has improved the laboratories' abilities to more accurately model complex physical phenomena thus improving their productive capability and reducing dependence on empirical scaling. This is particularly true in the design and testing of nuclear weapons and more recently in controlled nuclear fusion research. DOE programs in fundamental physical sciences are just beginning to use supercomputers as "experimental" devices for theoretical calculations. The need for large scale scientific computers is emerging in high energy, condensed matter, chemical and biological theory. Ab initio calculations for quark confinement, critical phenomena in alloy solidification and

superconductors, ground state properties of chemical mixtures, and properties of long-chain polymers are providing insight into the basic properties of matter. The Energy Science Advanced Computation subprogram will provide increased access to researchers for these areas of research, many of whom had to travel to Europe to obtain access to advanced computers.

The Supercomputing Research activity retains the traditional roles of the vendors, DOE laboratories, universities, and Government. The activity planned will expand the long range research program in advanced computer architectures, algorithms, and software. The development of advanced supercomputer mainframes will continue to be carried out by the vendors without direct Government support. The Government will continue to be a friendly buyer.

The DOE scientific research community comprises a large fraction of this country's expertise in large scale computational modeling. With sufficient support and coordination, major advances in this area can be made in this decade by combining the skills of mathematicians and computer scientists to maintain our leadership in understanding the basic principles required for future development of energy systems. Coordination with the scientific community and other Federal agencies is carried out by participation in the Interagency Committee on Extramural Mathematics Programs and Federal Coordinating Council on Science, Engineering, and Technology panels.

Recent accomplishments in this subprogram include the following:

o Five Future Supercomputer Research Machines Tested:

Initial tests have been completed on five research parallel processor systems that are being used to investigate a variety of approaches to the ultimate goal of simultaneous use of thousands of processors on a single problem. NYU/Courant Institute has a two processor ultracomputer prototype working. An eight processor dataflow prototype is running at MIT. A four processor-by nine memory device version of the Texas Reconfigurable Array Computer is running at the University of Texas. Los Alamos concluded an arrangement for leasing a Denelcor HEP-1 machine for the experimental computer program. They have already presented results of several physics problems on that machine and its availability in an open research environment should provide dramatic insight in concurrent processing on large scale DOE modeling problems. The new Cal Tech project started in FY 1983 is building on results already obtained on their four processor homogeneous machine. They have reported the calculation of theoretical masses of elementary particles on that system.

o Mathematical Analysis of Combustion Processes

The Applied Mathematics group at LBL reports significant improvements in the mathematical modeling of combustion processes and gas dynamics. Two recent PhD students have demonstrated numerical techniques for modeling turbulent combustion that predict phenomena not yet seen in experiments, including the effect of exothermic reactions and viscosity on the combustion of fuel in a closed chamber.

Supercomputing Research

This activity funds basic research at the national laboratories, universities, and private research institutions in three major categories: Analytical and Numerical Methods, Information Analysis Techniques, and Advanced Computing Concepts. In addition, experimental computing capabilities are being established as research facilities to support the exploration of new concepts in large scale scientific computing.

In FY 1985 an enhancement in the large scale scientific computing activity is planned, with emphasis on algorithms for large scale parallel architectures based on several experimental computer systems under study. This program will greatly accelerate the pace of projects in parallel supercomputing so that some of the research machines can be brought to a usable state as soon as possible. Also included in the plan is an expanded participation by interdisciplinary teams working on problem decomposition, algorithm development, numerical analysis, performance evaluation, and languages for highly parallel analysis.

In FY 1985 a total of $21,250,000 in operating funds, an increment of $6,580,000 over the FY 1984 level, is requested to expand the long range research program in large scale scientific computing.

An increment of $1,500,000 will be used to enhance the subactivity in Analytical and Numerical Methods. This subactivity supports the investigations of the fundamental properties of mathematical models used to simulate complex physical phenomena observed in energy systems. This category includes applied analysis, numerical methods for solving large systems of differential equations, and numerical analysis of algorithms.

The subactivity in Information Analysis Techniques will be expanded with an increment of $1,850,000. This subactivity supports the investigation of data management and statistical analysis of large scientific data sets common in DOE mission programs, such as High Energy Physics, Magnetic and Inertial Fusion, and others.

The subactivity in Advanced Computing Concepts will be expanded with an increment of $3,230,000 in order to provide additional research staff, graduate students, and engineering support for research machines being invesigated at universities and laboratories that have demonstrated viable designs for novel architectures. This activity meets a wide range of problems associated with the effective use of large scale scientific computers for modeling energy systems. The areas of research include software engineering techniques for design of quality mathematical software, display techniques for scientific data sets, and parallel architectures for high performance scientific computers. A variety of new techniques for decomposing large problems to execute on a large number of concurrent processors is being investigated in DOE laboratories and universities. These techniques will provide the insight needed to build the supercomputers of the 1990's.

These new architectures, employing several to perhaps hundreds or thousands of fast processors working concurrently to solve a single problem, require a thorough reexamination of all aspects of the solution method. Problems have to be decomposed into parallel parts for optimum execution. Algorithm characteristics such as accuracy, stability, robustness, and correctness of implementation must be investigated anew.

The R&D projects envisioned have two important facets requiring substantial cooperation and coordination among traditionally separate groups. One facet is the interdisciplinary teams of computational scientists, computer scientists, and mathematicians working on all aspects of large-scale scientific computing problems. Another facet is the cooperation of industry, government and universities on the design and engineering of several potentially strong candidate architectures.

The university researchers will play the major role in generating ideas and prototype software and in training graduate students in generating new applications. Government laboratory staff are in the forefront of tackling real world, large scale scientific problems and have unique resources for participating in these research projects. Industry likewise has a unique role in providing state-of-the-art production and testing facilities and would stand to reap great benefits in understanding future architecture and software issues that tend to limit industry use of supercomputers currently. The transfer of technology from the academic and laboratory research environment to industry would be as rapid as possible through these cooperative projects. The DOE program will be coordinated with the other agencies to share common facilities where possible, such as very large scale integration (VLSI) design facilities and component fabrication.

Energy Science Advanced Computation

The Office of Energy Research (ER) funds frontier research and development in many fields of science and engineering. ER has provided its research and development programs with state-of-the-art experimental facilities; however, most scientists in the ER programs (with the exception of magnetic fusion) have not had access to modern, large scientific supercomputers.

Because the ER scientists and engineers are located in DOE laboratories, universities, and industrial laboratories that are geographically dispersed throughout the country, the only practical solutions to the ER large-scale computing access problem are to establish a new network or to use an existing computer network. The network concept allows matching of computer resources to requirements across all ER programs rather than on an institution by institution basis.

As an interim solution to the ER computing problem, five percent of the Class VI computer time on the Magnetic Fusion Energy network was made available to other ER programs starting in May 1983. This does not represent a permanent solution because the MFE program currently has need for more computing capacity itself and the five percent of each of the two Class VI MFE machines satisfies only about ten percent of the ER program requirements. However, in the near-term, expansion of the MFE network to serve the additional ER users does represent a cost-effective solution.

For FY 1985, a total of $7,000,000 in operating funds is requested as a first step in expanding ER computing activities on the existing Magnetic Fusion Energy Computer Network to supply the large-scale computing needs of the High Energy and Nuclear Physics, Basic Energy Sciences and Biological and Environmental Research Programs.

Substantial data on the computing requirements of the Energy Research programs (with the exception of MFE) to be served by the network indicates that one additional state-of-the-art supercomputer system will satisfy those requirements in FY 1985. The costs associated with providing supercomputing resources for Energy Research scientists can be divided into the following three categories:

1. $3,500,000 for the lease and maintenance of the machine;
2. $1,500,000 for support staff to provide services for the broad spectrum of new users and applications;
3. $2,000,000 to expand the network communications and access facilities for these new users and to maintain the existing research computing facilities at the national laboratories.

In support of the operating program described above, $1,500,000 for capital equipment is needed for this subprogram in FY 1985. This request will permit the expansion of ER computing activities using the MFE Network to serve all Energy Research programs and will provide additional capital equipment for communications, peripherals and remote network access computing facilities. Specifically, $500,000 will be used for a hyper-channel and $400,000 for expanded disk storage. The remaining $600,000 will be allocated for communications equipment at selected energy research sites.

	FY 1983	FY 1984	FY 1985 Request
Engineering and Geosciences			
Operating Expenses	$ 17,200	$ 19,000	$ 20,795
Capital Equipment	1,120	1,150	1,500
Subtotal	18,320	20,150	22,295

This subprogram provides for the Department of Energy's principal long-term, fundamental research efforts in the disciplines of mechanical engineering and electrical engineering, as well as geology, geophysics and geochemistry. Topics are chosen for funding for their long-term importance to meeting the Nation's energy needs.

The FY 1985 request provides for continuing the principal lines of research now underway and for increasing by about ten the number of scientists and engineers anticipating in these important aspects of energy research.

In addition to the requests for operating funds discussed more fully in the next several paragraphs, $1,500,000 is requested for capital equipment including, for example, prototype remote handling equipment for research on intelligent control systems at Oak Ridge National Laboratory, and telemetry and computer interfacing equipment to link existing seismic networks and the new Center for Computational Seismology at Lawrence Berkeley Laboratory. The request for capital equipment is 7.2 percent of the request for operating funds which experience has shown is the minimum level for effective research in continuing projects and for meeting the critical needs for the work to be initiated in FY 1985.

Engineering Research

To meet the long term basic research needs of energy technologies and of industry Engineering Research pursues two goals: 1) to broaden the technical and conceptual base for solving future engineering problems in the energy technologies, and 2) to extend the body of knowledge underlying current engineering practice in order to open new ways for enhancing energy savings and production, prolonging useful equipment life, and reducing costs while maintaining output and performance quality.

All the energy technologies benefit from fundamental advances in the areas emphasized in Engineering Research. For instance, improved basic understanding of heat transfer is pertinent to all known energy technologies. Such advances are essential to ensure flexibility in meeting the Nation's future energy needs.

With the advent of inexpensive, compact computer hardware and powerful new analytical methods for nonlinear problems, generic energy related engineering research is generated increasing opportunities for significant advances. Those advances have the potential not only for valuable, even revolutionary changes in future energy systems, but also for major improvements in energy utilization and production in the next few years. This is signaled by both the pressure of proposals with important new ideas and the achievements to date of this relatively new activity.

This activity seeks the knowledge and data bases needed for reliable and economical implementation of computer aided energy engineering. Specific fundamental areas addressed are 1) Mechanical Sciences - including tribology, heat transfer, fluidized beds, and solid mechanics; 2) System Sciences - including process control, and instrumentation; and 3) Engineering Data and Analysis - including nonlinear dynamics, and data bases for energy engineering systems.

Recent accomplishments in Engineering Research include:

- o The discovery of fatigue induced surface oxidation as an important mechanism for wear of unlubricated metal surfaces sliding in close contact, a potentially catastrophic condition inside machinery.

- o Initial research on integrated thermionic circuits with an unexpectedly early application to fast computer terminal displays.

In FY 1985 at the request level for Engineering Research, $7,115,000, an increase of $765,000, support of carefully selected, generic, high quality engineering research in the existing program areas enumerated above will be maintained.

Most of the requested increment will be applied to studies of energy related nonlinear systems which continue to pose challenges to both research oriented engineers and their practicing colleagues. Current design practice, based on research conducted as long as 20 years ago, and the design tools then available, continues to be limited by the assumption that many systems do operate at nearly linear conditions. Indeed, they do

not, but the tools and understanding to handle the more complex nonlinear conditions have not been available. There is little if any understanding of the dynamic response of these large-scale, nonlinear, distributed parameter systems. Recent relevant developments in applied mathematics and great advances in experimental techniques offer important new research opportunities in this field. Exploitation of these opportunities is essential for improving the performance of many of the nation's energy systems.

Geosciences

To meet the Department's long-range needs for earth science information, the Geosciences activity supports research in geology, geophysics, geochemistry, rock mechanics, tectonophysics and solar-terrestrial physics.

This research is carried out principally at the DOE national laboratories and at universities. All of the projects are chosen for their special significance to present and future energy technologies. For example, coordinated projects in nuclear waste isolation and Continental Scientific Drilling address long-range national energy concerns. Studies of the temperature and tectonic history of subsiding basins are leading to a better understanding of the development of energy resources in nature and thus to their more effective exploitation. Development of new geophysical methods and of computer codes for improved modeling of geophysical data and their use in resource exploration are leading to improved methods of locating resources, modeling the earth's crust and identifying sites for nuclear waste isolation.

Geochemical studies of element migration and energy and mass transfer are providing the knowledge base needed to understand the mechanisms of energy and mass transfer in hydrothermal systems, the potential migration of radio-nuclides from a repository, and the concentration and location of mineral resources. Research in organic geochemistry is yielding an improved understanding of the origin, development and emplacement of gas, oil, and coal deposits, is identifying the sources of pollutants in these resources and may suggest ways of dealing with them. As the traditional sources of energy diminish, alternatives must be found. Further, the extraction and use of energy resources result in wastes, the safe disposal of which requires a thorough knowledge and understanding of the earth's structure and processes which, in turn, requires continued fundamental research. The development of an adequate base of knowledge in the geosciences is therefore critically needed for energy resource recognition, evaluation and utilization.

Recent Geosciences accomplishments include the following:

- Basic data on sound waves have led to discovery of a new approach to monitoring recovery of heavy oils. Results from studies at Stanford University show that very large reductions in acoustic wave velocities (50 percent) and wave amplitude (6 fold) occur upon heating heavy oil sands under in situ pressure conditions, and that the low frequency dielectric constant of rock is a very strong indicator of the water content. These results form the basis for remotely monitoring enhanced oil recovery. A field test of this approach to geophysical monitoring is being sponsored by the oil industry.

- A newly designed device to measure convective heat flow within a wellbore has been tested by Sandia National Laboratory scientists. This instrument represents a significant achievement in thermal measurements in boreholes, as previous measuring techniques could not distinguish between conductive and convective heat flow components. This new device functions by thermally perturbing the convecting medium and measuring the response of the medium to the perturbation. The rate of decay of the thermal pulse is related to the ground water velocity vector.

The request for FY 1985 operating expenses for the Geosciences of $13,680,000 provides for support of the geosciences activities in DOE along lines for which the scientific priority is high and which bear directly on the long range research needs of the Department. The $1,030,000 increase over FY 1984 will be used for limited strengthening of ongoing efforts.

The thermal regimes portion of the cooperative interagency Continental Scientific Drilling Program will be maintained with geophysical studies, but without the option for intermediate depth drilling in the geographic areas under study in the thermal regimes part of the national program (Valles Caldera and Long Valley).

This program has attracted substantial interest and support from industry and academia and the portions dealing with thermal regimes is especially appropriate for support by the Department of Energy. The other cooperating agencies are NSF and USGS. The increase requested for the Geosciences in FY 1985 will provide for strengthening of research on downhole techniques for operation in a very hostile environment (corrosive, and at high temperatures and pressures).

Advanced Energy Projects	FY 1983	FY 1984	FY 1985 Request
Operating Expenses	$ 8,300	$ 9,100	$ 10,810
Capital Equipment	290	310	320
Subtotal	8,590	$ 9,410	$ 11,130

The objective of the Advanced Energy Projects subprogram is to explore the feasibility of novel, energy-related concepts, as they evolve from basic research. Such concepts are at an early stage of scientific definition and therefore would not qualify for support by technology programs. Because they are new and untried, those concepts invariably represent a high risk; to qualify for support they must also have the potential for an eventual high pay-off. Also supported is exploratory research on concepts that do not fit easily into the existing Department of Energy program structure. An area of major programmatic attention is the transfer of successful projects to proper technology programs; such transfers now are effected every year.

Support of exploratory research on novel concepts of the type described above is needed to provide the seed for technical innovation. However, such research does not generally qualify as basic research, where the objective is to gain knowledge and understanding of processes and phenomena in nature. Neither does it qualify as technology-related: the link with any specific technology needs yet to be established. Hence, the Advanced Energy Projects subprogram fills a very real void between basic and technology-related research.

Thus, for example, two novel approaches to controlled fusion--very different from those currently pursued--have been proposed as a result of basic research in elementary particle physics. Both muon-catalyzed fusion and quark-catalyzed fusion are being actively explored under Advanced Energy Projects sponsorship.

The mode of operation for this interdisciplinary, and still relatively new, subprogram is to support individual projects for a limited time only; it differs from other subprograms in that it does not fund ongoing evolutionary research. The spectrum of projects supported is very broad, encompassing, for example, the development of new sources of electromagnetic radiation, new methods of better fossil fuels utilization, totally new approaches to controlled fusion and new approaches to solar energy collection and utilization, just to name a few. Close contact is maintained with DOE technology programs to ensure proper coordination. Projects are selected on the basis of unsolicited proposals received from researchers at universities, industrial laboratories (especially small R&D companies) and national laboratories. At present, about forty projects are being supported, which allows a turnover rate of about fourteen projects a year. A recent accomplishment of Advanced Energy Projects is the measurement, for the first time, of fusion reaction rates in a scheme utilizing mu mesons as reaction catalysts. Even though the practicality of the scheme for power generation remains questionable, mainly because of the high cost of producing mu mesons, the demonstrated high reaction yield may lead to other applications, such as high-intensity neutron sources.

Last year continued to bring evidence of a wide recognition of Advanced Energy Projects as an important vehicle in promoting science-based technical innovation:

- In March 1983 the American Physical Society held its first Symposium on Advanced Energy Projects. All five invited speakers were Principal Investigators on projects supported by this subprogram.
- The annual Energy Technology Conference and Exposition held in Washington, D.C. in February 1983, devoted a special session to Advanced Energy Projects. Speakers at the session were Principal Investigators on projects supported by this subprogram.
- Articles describing Advanced Energy Projects appeared in journals such as Chemical & Engineering News, and Physics Today.
- On the initiative of Advanced Energy Projects a Symposium on Novel Sources of Electromagnetic Radiation was held in Germantown, Maryland in April of 1983. The symposium reviewed recent progress in areas such as x-ray lasers, free electron lasers, etc. Advanced Energy Projects is the Department of Energy's focal point for support of non-defense related work in this field.

The FY 1985 request for the Advanced Energy Projects subprogram is $10,810,000 in operating expenses and $320,000 in capital equipment funds. The funding level translates directly into the number of projects which this subprogram will be able to start each year; that is, the number of new concepts which will be given a chance of being explored in some depth. The increase requested will maintain the total number of projects supported at any given time at last year's level of about forty; with a typical turnover period of three years, this translates into about fourteen new starts in FY 1985. In addition, the subprogram will develop, on a modest scale, a new initiative in exploring novel sources of electromagnetic radiation such as optical klystrons, x-ray and gamma-ray lasers and free electron lasers. A need for such an initiative has been pointed out in a report of the Symposium on Novel Sources of Electromagnetic Radiation (April 21-22, 1983).

	1983	1984	1985 Request
Biological Energy Research			
Operating Expenses	$ 9,500	$ 10,580	$ 12,490
Capital Equipment	370	400	560
Subtotal	9,870	10,980	13,050

The objectives of the Biological Energy Research subprogram are a) to develop an understanding of fundamental biological phenomena in plants and microorganisms that will underpin the development of improved strategies for enhanced productivity of renewable resources; b) to generate a base of fundamental information on which to construct new and improved microbiological conversions of materials into useful fuels and chemicals; and c) to explore and understand basic biological phenomena which may be employed in developing biosystems as substitutes for energy intensive chemical processes.

The general area of biotechnology has been identified worldwide, along with computer technology and robotics, as one of the most promising areas for future technology development. The basis of that projection derives in large part from the almost explosive recent development in capabilities for manipulating genetic materials. These capabilities have their foundation almost exclusively on advances made in basic biological understanding primarily in molecular genetics. It is equally apparent that the application of biotechnology will remain greatly dependent on continuing advances in fundamental areas of biology including physiology, biochemistry and genetics. Recognition of the promise of payoff from enhanced plant science research was provided in a recent OSTP-COSEPUP (Committee on Science, Engineering and Public Policy) report, "Research Briefings for OSTP, NSF and Selected Federal Departments and Agencies."

Biotechnology may be expected to impact the energy sector in a number of ways. Clearly the use of biological renewable resources is growing and the future improvement of green plant productivity employing genetic engineering and other cellular techniques is almost assured. Likewise in the fermentation of renewable resources to useful fuels and chemicals there is high promise that new biotechnology will be developed. A number of potential biotechnological systems have been proposed for amelioration of pollutants emitted in combustion. In addition a number of potential biotechnological systems have been proposed for preprocessing of fuels for cleaner combustion. There is growing activity aimed at utilizing microbial systems either directly or indirectly as part of enhanced oil recovery techniques. Further, the use of biosystems for displacing energy intensive chemical systems as an energy conservation measure are options that are receiving more attention. The speed with which each of these developments will occur is dependent on a number of factors including continuing advances in the information base, the price of energy supplies and the attractiveness of other features of biotechnology.

The Biological Energy Research subprogram is the only program in the Federal Government specifically aimed at generating the basic biological information in support of energy biotechnology development. The subprogram covers work in the plant and microbiological sciences almost exclusively. The research covers fundamental studies on the light energy conversion process of photosynthesis, basic processes of plant growth and development, the effects of stress on plants, studies to understand the adaptive mechanisms plants have developed to survive under suboptimal conditions, the basic processes of genetic transmission and expression of characters in plants, how plants manage the energy that is trapped photosynthetically with respect to metabolic pathways and localization of products, the basic patterns of regulation of biochemical pathways in plants and how plants interact with other organisms with respect to pathogenicity, symbiosis and other molecular and cellular interplays.

Microbiological studies encompass work on basic studies of a variety of fermentation pathways leading to fuel and chemical production, microbial degradation of lignin, hemicelluloses and cellulose, the biological basis of methanogenesis; and how microorganisms deal physiologically and biochemically with harsh conditions, e.g., extremely high temperatures and total absence of oxygen (anaerobicity). The program emphasizes the genetics of little studied, but important, microorganisms in bioconversions, how microbes interact and form consortia to carry out complex metabolic conversions, and regulatory mechanisms that determine how the organisms grow and produce particular chemical products.

A major share (75%) of the work is conducted at university laboratories, the remainder is located at national laboratories.

Some representative recent accomplishments include:

- For the first time it has been possible to quantitate genetic transposition (movement of genes within the genome) in a higher organism. This was done in maize by following the frequency of movements among male fertility restorer genes in male sterile lines.

- The gene coding for susceptibility to the herbicide atrazine in plants has been identified, cloned and sequenced. A mutant gene which is responsible for resistance to the herbicide activity has likewise been studied. The difference between the two is simply one nucleotide in the DNA sequence.

- Agrobacterium Ti plasmid, a DNA segment found in a bacterium has now been used to introduce alien genes into higher plants. The unwanted side effect of this plasmid, namely tumor formation in the recipient plant, has been abolished by eliminating one gene of the plasmid responsible for the effect.

- Stomata are tiny pores in the surfaces of leaves which control the entry and exit of gases (carbon dioxide, water, oxygen) to the interior cells of the leaves where photosynthesis occurs. Guard cells are cells that are part of the stomatal structure regulate the opening and closing of the pores and thus regulate photosynthesis. It has now been shown for the first time that individual guard cells may be studied using innovative microtechniques to gain a better understanding of regulatory behavior in guard cells.

There has been a significant increase in interest on the development of biotechnology in the industrial, university and federal components in the U.S. While industry has taken the lead in bringing on the commercialization of processes, there is a major role of the federal supported research network at universities and other laboratories to sponsor and conduct the vast amount of fundamental research requisite for any substantial industrial development of biotechnology.

The FY 1985 request for Biological Energy Research is $12,490,000 in operating and $560,000 in equipment. This represents a level which provides for a continuation of current activities. Specific areas of continued emphasis in FY 1985 will include:

- Investigations on the molecular and cellular aspects of stress in plants, and studies in plant regulatory mechanisms,

- Investigations on microbial interactions in bioconversions. In addition, interdisciplinary research in plant science and microbiology will receive some attention.

This level would allow a response to some of the numerous new proposals for very high quality research in these areas aimed at providing much needed fundamental information on which to base the nation's growing biotechnology industry.

This level of funding could also begin to address a need in the plant and microbial sciences, namely:

Establishment of interdisciplinary collaboration - the extremely impressive advances in genetic manipulation techniques will not be exploitable optimally unless there is parallel progress in the basic understanding of the characters which might be modified in plants and microorganisms. The complexity of biological systems is increasingly demanding the use of new and often more sophisticated techniques of physics and chemistry. Most investigators do not possess expertise in multiple areas. BER plans to initiate a very small number of interdisciplinary research groupings which focus on key plant and microbial science problems. These include studies on interactions of roots and soil, and metabolic regulation and the biosynthesis of important molecules. Only with an increasing injection of the more physical-chemical analytical approaches will it be possible to capitalize on the techniques of recombinant DNA and cell and tissue cultures to gain the depth of understanding needed in the plant and microbial sciences.

DOE is especially well equipped to pursue such interdisciplinary ventures because of its existing extraordinary strength in these areas as well as the flexibility available for organizing such groupings. The interdisciplinary initiatives would complement, not duplicate, research activities supported by the NSF and USDA.

	FY 1983[a/]	FY 1984	FY 1985 Request
Program Direction			
Operating Expenses	$ 3,170	$ 3,970	$ 3,830
Total FTE's	56	62	62

a/ Reflects comparability adjustment of 1 FTE and $70,000 from Magnetic Fusion Energy in connection with Applied Mathematical Sciences Research.

The FY 1985 request for Basic Energy Sciences Program Direction is $3,830,000, a decrease of $140,000 from the FY 1984 level. These funds are required to provide for the salaries, benefits, travel and related expenses associated with 62 full-time equivalents. This funding level represents a number of management savings while at the same time absorbing the increased personnel costs related to continuation of the FY 1984 staffing level. The increased workload resulting from growth in selected areas of the basic research program, management of the expanding Small Business Innovation Research Program (SBIR), and absorption of the expanded effort to meet the Department's future large-scale scientific computing requirements will require a considerable increase in staff productivity and more efficient management and coordination activities among the Headquarters, field, and contractor staffs.

Basic Energy Sciences is a broadly diversified program responsible for mission-oriented research, the chief purpose of which is to provide the fundamental scientific and engineering base on which the Nation's future energy options depend. Its staff must possess expertise covering many subfields in the areas of chemistry, physics, engineering, metallurgy, applied mathematics, geosciences and biology, as well as in administration, procurement and financial management. The staff is responsible for development, direction, and management of complex technical programs, each involving one or more of the scientific areas mentioned above. Their activities include assessing scientific needs and priorities of the program, developing long-range program plans, technical review of proposals from laboratories and universities, and monitoring the progress of ongoing university contracts, laboratory programs, and construction projects.

It is extremely important to appreciate the diversity and scope of the research effort involved in the Basic Energy Sciences program. In FY 1984, for example, approximately 1,300 research projects will be underway either at agency laboratories or at more than 150 colleges or universities in 45 states. Research projects are expected to increase in FY 1985. Evaluation, monitoring and management of this large number of diverse projects primarily from the Headquarters requires frequent contact with the contractors and laboratory staff and involves numerous workshops, planning meetings, and project reviews throughout the year.

During recent years research projects at universities have increased from 18 to 26 percent of the BES budget, and the workload per university project is significantly greater than that for a laboratory project. This is especially true with regard to evaluation of proposals, of which approximately 10 percent of those reviewed result in new contracts each year. A stable staff is required to maintain a strong core program; to evaluate research programs which have continued to grow in recent years in newer emerging priority areas having great potential importance to energy; to oversee management, operation, and ongoing construction of unique research facilities; and to promote early application of the results of this basic research.

In addition to the ongoing basic research program, the three-phase Congressionally mandated SBIR program (Public Law 97-219) will be entering its third year. Phase I was implemented in FY 1983 with 9,000 solicitations mailed, resulting in 1,734 proposals spread among 25 technical topics. There were 106 contracts awarded totaling over $5,000,000. The first year of operation resulted in heavier than anticipated workload with extensive overtime and assistance outside the SBIR staff. Workload in FY 1984 will increase even further as all 106 of the initial contractors are expected to submit proposals to enter Phase II of the program and new Phase I awards are also made. During FY 1985 the initial FY 1983 projects will enter the second year of Phase II, FY 1984 projects will enter their first year of Phase II, and new Phase I projects will begin. This results in substantial increases in the number of proposals to be processed and evaluated, increased procurements and projects to be monitored and evaluated, site visits for those projects entering Phase II, and increases in the number of debriefings requested by contractors not receiving awards.

Furthermore, this program now funds the scientific computing staff established to manage the newly assigned responsibilities related to large-scale scientific computing. This staff will manage two important activities related to large-scale scientific computing. Those activities are: (1) providing access to large computers for the researchers supported by the scientific programs of the Office of Energy Research; and (2) support of research in scientific computing necessary to meet the Department's long-range needs. Specific workload includes managing a number of research projects, including conducting peer reviews and evaluating proposals, performing economic and cost benefit studies and analyses of user needs, managing the Magnetic Fusion Energy computer network, and providing a single DOE focal point to maintain liaison with other Federal agencies, universities, and other concerned organizations.

Management Initiative

This decision unit reflects $3,000,000 for savings resulting from management initiatives in the area of administrative processes/field structure.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
BASIC ENERGY SCIENCES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: General plant projects

2. Project No.: 85-ER-400

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 2nd Qtr. FY 1985

4. Date construction ends: 4th Qtr. FY 1986

5. Previous cost estimate: None
Date:

6. Current cost estimate: $5,750
Date: 6/83

7. Financial Schedule:

Fiscal Year	Obligations	Costs			
		FY 1983	FY 1984	FY 1985	After FY 1985
Prior Year Projects	$ 300	$ 100	$ 0	$ 0	$ 0
FY 1983 Projects	300	200	100	0	0
FY 1984 Projects	400	0	300	100	0
FY 1985 Projects	5,750	0	0	2,300	3,450

8. Brief Physical Description of Project

This project is required to provide for minor new construction, other capital alterations and additions, and for buildings and utility systems. Where applicable, the request also includes the cost of installed capital equipment integral to a subproject. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may be expected to result in additions, deletions, and changes in the currently planned subproject. In general, the estimated funding for each location is preliminary in nature, and is intended primarily to indicate the relative magnitude of the requirements. No significant R&D program is anticipated as a prerequisite for design and construction of the subprojects under construction.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: General plant projects

2. Project No.: 85-ER-400

8. Brief Physical Description of Project (continued)

Included in our request for the first time in FY 1985 is full GPP funding for the Argonne National Laboratory. Previously, landlord responsibility at this laboratory has been with the Nuclear Energy - Breeder Program, but program shifts and restructuring necessitates the shift of this responsibility to the BES program.

Due to the recent budget constraints placed on the Breeder Program, the normal GPP requirements at the Argonne National Laboratory have deteriorated to the point that a major budget increase is required in FY 1985 to meet minimal laboratory requirements.

The currently estimated distribution of FY 1984 funds by office is as follows:

Argonne National Laboratory	$ 5,000
Ames Laboratory	600
Notre Dame Radiation Laboratory	50
Stanford Synchrotron Radiation Laboratory	100
Total project cost	$ 5,750

9. Purpose, Justification of Need for, and Scope of Project

The following are examples of the major items to be performed at the various locations. Since needs and priorities may change, other projects may be substituted for the examples listed below, and some of these may be located on non-Government owned property.

Argonne National Laboratory

Group I - Rehabilitation Projects - ANL-West

1. Replacement of Underground Steam and Condensate Piping
2. Rehabilitation of Industrial Waste and Drainage Ditches
3. Replacement of Power Poles

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: General plant projects — 2. Project No.: 85-ER-400

9. Purpose, Justification of Need for, and Scope of Project (continued)

Group II - Rehabilitation Projects - ANL-East

1. Replacement of Water Chiller, Bldg. 202
2. Rehabilitation of Sewer System
3. Replacement of Water Chiller, Bldg. 205

Group III - Upgrade/Programmatic Projects

1. Thermochemical Properties Laboratory, Bldg. 205
2. Storage Building for EBR-II Water Treatment Chemicals, ANL-West
3. Upgrading of Variable Temperature Rooms, Bldg. 202

ANL allocates 50% of its GPP funds to plant rehabilitation and 50% for upgrading and programmatic projects. Given the relative size and condition of its two sites, ANL allocates 12.5% to ANL-West and 37.5% to ANL-East for rehabilitation projects. FY 1985 GPP funds of $7.0 million would thus allocate approximately $0.9 million to Group I, $2.6 million to Group II, $3.5 million to Group III.

At present, a total documented GPP backlog of $20.7 million exists, consisting of $1.2 million for ANL-West rehabilitation (Group I), $4.8 million for ANL-East rehabilitation (Group II) and $14.7 million for required upgrading and programmatic projects at both sites. Surveys made at both sites indicate that rehabilitation needs are fare more extensive; only those needs which are most critical are included in the above backlog. This backlog is not static and is constantly under review by ANL management so that the most critical requirements are taken care of as promptly as possible with available GPP funding. These requirements may come about as the result of the unscheduled failure of major plant components or the need to satisfy scientific program requirements. A recent example of unanticipated system plant component failures was the recent destruction of the roof over the Hot Fuel Examination Facility at ANL-West in a recent storm which required an immediate shifting of ANL priorities to provide the necessary construction funds for replacement of the roof.

The backlog of GPP projects has tended to increase steadily in recent years due to the shortfall in funding line item requests for plant rehabilitation at ANL-East and ANL-West, and because of programmatic shifts at ANL which have required modifications to the existing plant. When it is considered that total GPP funds available to ANL in FY 1983 and FY 1984 total only $2.1 million, it is readily apparent that ANL needs are far outpacing the availability of funds with which to satisfy them.

1. Title and location of project: General plant projects — 2. Project No.: 85-ER-400

9. Purpose, Justification of Need for, and Scope of Project (continued)

Ames Laboratory..... $ 600

Requirements include for example: renovation of obsolete radioactive facilities; upgrading piping and pumps in the central steam plant; and energy conservation and safety components.

The probjects described will be constructed on the Ames Laboratory, non-Government owned property.

Notre Dame Radiation Laboratory..... $ 50

Requirements include minor building modifications to properly house staff members and to make optimum use of laboratory research space.

The probjects described will be constructed on the Notre Dame Radiation Laboratory, non-Government owned property.

Stanford Synchrotron Radiation Laboratory..... $ 100

Requirements include a necessary safety upgrade of the hazardous gas exhaust system and an optics evolution laboratory for evaluation of the surface quality of mirrors before and after coating.

The probjects described will be constructed on the Stanford Synchrotron Radiation Laboratory, non-Government owned property.

10. Details of Cost Estimate

See description, item 8. The estimated costs are preliminary and, in general indicate the magnitude of each program. These costs included engineering, design, construction and inspection.

11. Method of Performance

Design will be on the basis of negotiated architect-engineer contracts. To the extent feasible, construction and procurement will be accomplished by firm fixed-price contracts and subcontracts awarded on the basis of competitive bidding.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
BASIC ENERGY SCIENCES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Accelerator improvements and modifications, various locations

2. Project No.: 85-ER-401

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 1st Qtr. FY 1985

4. Date construction ends: 4th Qtr. FY 1986

5. Previous cost estimate: None
Less amount for CP&D: None
Net cost estimate: None
Date:

6. Current cost estimate: $2,400
Less amount for CP&D: 0
Net cost estimate: $2,400

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1985	$ 2,400	$ 2,400	$ 2,400	$ 1,000
1986	0	0	0	1,400

8. Brief Physical Description of Project

This project provides for additions and modifications to accelerator and reactor facilities, which are supported by the Basic Energy Sciences program. Since program priorities and needs change, the projects described below indicate the most likely projects to be funded. A continuing evaluation, however, is necessary to ensure that those projects with the greatest productivity are funded. Three projects at the Brookhaven National Laboratory are requested to incorporate improvements at the High Flux Beam Reactor and the National Synchrotron Light Source.

Three projects are requested at the Oak Ridge National Laboratory for improvements at the Bulk Shielding Reactor, Holifield Heavy Ion Facility, and at the High Flux Isotope Reactor. In addition, one project is requested at the Argonne National Laboratory for modifications at the Atlas accelerator.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Accelerator improvements and modifications, various locations

2. Project No.: 85-ER-401

9. Purpose, Justification of Need for, and Scope of Project

The following are the projected items of work to be performed at the various locations. Since needs and priorities may change, other projects may be substituted for the examples listed below, and some of these may be located on non-Government owned property.

Brookhaven National Laboratory

High Flux Beam Reactor Facility (HFBR)..... $ 500

Funds are requested to assure the safe and efficient operation of the HFBR. Funds requested will be used for monitoring devices within the reactor, electronic transducers, process recorders, and emergency generators.

National Synchrotron Light Source (NSLS)..... $ 1,200

Funds requested are for the total NSLS research facility which needs annual modifications, improvements and additions. Included are improvements for the: replacement components for X-ray and VUV lines, beam diagnostic devices, power supplies, vacuum, RF systems, and magnet systems. In addition, improvements will be made at the x-ray ring of the NSLS facility in order to establish a capability for atomic physics research. The main components to be added are a radiation enclosure and a photon analysis system consisting of a monochromator, a mirror for x-rays and a high vacuum pumping system, all of which will be coupled to the x-ray ring. The improvement will allow for study of the interaction of intense, high energy x-rays with atoms and ions. These will improve the performance of the NSLS and therefore will enhance the usefulness of the facility for basic research.

1. Title and location of project: Accelerator improvements and modifications, various locations

2. Project No.: 85-ER-401

9. Purpose, Justification of Need for, and Scope of Project (continued)

Oak Ridge National Laboratory

High Flux Isotope Reactor (HFIR)..... $ 300

This project will provide for improvements to those portions of the Critical Experiment Facility used to perform safety related reactivity measurements required by the High Flux Isotope Reactor (HFIR) Technical Specifications on all new HFIR fuel assemblies by replacing obsolescent facility safety and operating instrumentation with new instrumentation, and adding capability which will permit the required measurements to be made in the subcritical code. These measurements are safety related and are required to ensure compliance with the HFIR Technical Specifications. The presently installed safety and operating instrumentation is almost entirely early model vacuum tube equipment, some of it up to approximately 30 years old and difficulties are anticipated in maintaining and spare parts for this equipment as it ages further. Therefore, replacement of this obsolescent instrumentation with up-to-date equipment will help enhance future reliable operability of this facility.

Bulk Shielding Reactor..... $ 200

Funds requested are for slight modifications of the neutronics characterization through the reconfiguring of reflector and absorber components so that the research program will have access to the highest neutron flux available.

Argonne National Laboratory

Atlas Accelerator..... $ 200

The ANL ATLAS accelerator will be modified to incorporate a beam line for atomic physics research. A beam of selected heavy, multiply charged ions traveling with high velocities will be made available by the modifications and will allow study of interactions of these ions with atoms, other ions, molecules, electrons and photons. Knowledge important to energy technologies, especially magnetic fusion, as well as depended understanding of physics are expected. The principal components of the beam line are magnetic quadrupole focusing elements, control slits, beam profile monitor, steering plates and Faraday cups. An all metal high vacuum system pumped principally by two cryopumps and one ion pump will be installed. Electronic and power supplies associated with these elements will be added.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Accelerator improvements and modifications, various locations

2. Project No.: 85-ER-401

10. Details of Cost Estimate

a.	High Flux Beam Reactor Facility	$ 500
b.	National Synchrotron Light Source	1,200
c.	High Flux Isotope Reactor	300
d.	Bulk Shielding Reactor	200
e.	Atlas Accelerator	200
	Total Project Cost	$ 2,400

11. Method of Performance

Design, engineering, and inspection will be performed by laboratory staff. To the extent feasible, construction and procurement will be accomplished by fixed-price subcontracts awarded on the basis of competitive bidding.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
BASIC ENERGY SCIENCES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Stanford Synchrotron Radiation Laboratory Enhancement
Stanford Linear Accelerator Center
Stanford, California

2. Project No.: 85-ER-402

3. Date A-E work initiated: 1st Qtr. FY 1984

3a. Date physical construction starts: 2nd Qtr. FY 1984

4. Date construction ends: 4th Qtr. FY 1986

5. Previous cost estimate: $12,930

6. Current cost estimate: $13,030
Less FY 1983 PE&D: 100
$12,930
Date:

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1984	$ 1,240	$ 1,240	$ 1,240	$ 1,240
1985	11,690	9,130	9,130	8,630
1986	0	2,560	2,560	3,060

8. Brief Physical Description of Project

The Stanford Synchrotron Radiation Laboratory (SSRL) Enhancement will be located at the Stanford Synchrotron Radiation Laboratory. SSRL is colocated with the Stanford Linear Accelerator Center (SLAC) on Stanford University property that has been leased to the Department of Energy.

The SSRL Enhancement project will include the construction of new conventional and research facilities and the alteration of and additions to existing facilities for the purpose of providing ultra-high brightness synchrotron radiation from insertion devices (wigglers and undulators).

The project is divided into three major portions: (a) construction of two beam lines, one on the SLAC Positron Electron Project (PEP) storage ring and one on the SLAC SPEAR storage ring; (b) alteration of the electron storage ring SPEAR for high flux synchrotron radiation research and (c) construction of three conventional facilities: a PEP Beam Line Facility (PBF) (3,500 GSF), a Light Assembly Shop (LAS) (8,600 GSF), and a Laboratory/Office Building (LOB) (19,800 GSF).

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Stanford Synchrotron Radiation Laboratory Enhancement
Stanford Linear Accelerator Center
Stanford, California

2. Project No.: 85-ER-402

8. Brief Physical Description of Project (continued)

SSRL Conventional Construction

The site at PEP chosen for the PEP Beam Line and the associated facility -- (PBF) is just within the existing SLAC lease boundary and it will not be necessary to acquire more land from the University for the facility. The site requires a retaining wall for the access road, service yard, and PBF building which will be half buried into the PEP ring earth shielding mount. The PBF will be an experimental hall with three adjoining rooms and partial mezzanine. The Light Assembly Shop (LAS) will consist of a Vacuum Clean Room, and Vacuum Shop Office, a Beam Line Component Assembly Shop, a small Machine and Welding Shop, a Machine Shop Office, a Beam Line Component Storage Deck, and support rooms. The Library/Office Building (LOB) will be a two story building. The upper floor will provide up to 43 offices, a library, a conference room, a drafting room, a lounge-kitchen area; seven work rooms and two HVAC equipment rooms. The ground floor will provide a receptionist area, two large work rooms, up to 24 offices, an x-ray lab, a meteorology lab, a VUV lab, an electronics lab and four lab storerooms.

The optimum location for the LOB is presently occupied by an existing SLAC liquid hydrogen facility which SSRL will relocate to a new site selected by SLAC.

Special Facilities

A 26-period, 2-meter rare-earth cobalt undulator magnet will be installed on the PEP storage ring to produce photon beams peaked at 13 KeV. A scattering beam line will originate with a 54-pole rare-earth cobalt wiggler magnet. Machine improvements will include reduction of SPEAR emittance and vertical aperture, beam stabilization, and a new LINAC electron injection system.

9. Purpose, Justification of Need for, and Scope of Project

Over the past decade, the development of synchrotron radiation has led to major advances in a number of different scientific and technological fields, but particularly materials science, condensed matter physics and chemistry, as well as the biological sciences. Each order of magnitude increase in photon flux or spectral brilliance achieved during this period has resulted in qualitatively new experiments which provide previously unobtained information and yield new understandings.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Stanford Synchrotron Radiation Laboratory Enhancement
Stanford Linear Accelerator Center
Stanford, California

2. Project No.: 85-ER-402

9. Purpose, Justification of Need for, and Scope of Project

The most significant recent advances in photon flux and brilliance have been, or will be, the result of: (a) the development of insertion devices (wigglers and undulators) at SSRL and (b) improvements in storage ring characteristics (reduction of emittance and increases in current).

As a result, new storage rings are presently being planned which are optimized for high spectral brilliance and photon flux through utilization of insertion devices, rather than bending magnets, for the production of radiation and through the achievement of extremely low emittances and high currents. These rings are also optimized for specific spectral regions through choice of stored electron energies. Generally, stored electron energies at 1.0 to 1.5 GeV are utilized for ultra-high brilliance soft x-ray and vacuum ultraviolet (VUV) generation whereas rings of greater than 3.0 GeV are used for ultra-high brilliance x-ray generation.

The SSRL improvements described here will rapidly and economically yield major increases in the photon flux and spectral brilliance available at SSRL in all spectral ranges. In addition, x-ray spectral brilliance far beyond those achieved or proposed elsewhere in the world will be obtained. The SSRL construction will also increase the time available for dedicated synchrotron radiation operation of the storage ring SPEAR and increase the effectiveness of utilization of the radiation. At the same time, it will provide for testing and development of individual insertion devices as well as the techniques for utilizing many insertion devices on one storage ring.

The existing Stanford Synchrotron Radiation Laboratory has outstanding user facilities that can be dramatically and quickly improved in the hard x-ray region, thereby providing researchers with unparalleled photon brightness over an extended portion of the electromagnetic spectrum. A past 100-fold improvement to SSRL intensity in the soft x-ray region involved the installation at SPEAR of a permanent magnet undulator conceived and built at LBL. A current LBL/SSRL collaboration will provide a 50-fold improvement over the entire energy range based on an LBL-developed wiggler. Therefore, it is logical to continue joint activities to further improve SSRL facilities as a cost-effective way of providing researchers with additional advanced tools to complement those available elsewhere.

This project will be constructed at the Stanford Linear Accelerator Center which is non-Government owned property.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Stanford Synchrotron Radiation Laboratory Enhancement
Stanford Linear Accelerator Center
Stanford, California

2. Project No.: 85-ER-402

10. Details of Cost Estimate

(a)	Engineering, design, inspection and administration...	1,930
(b)	Construction costs.....	8,360
(c)	Standard equipment.....	230
(d)	Removals and relocations.....	0
(e)	Contingencies at approximately 19% of above.....	2,410
TOTAL ESTIMATED COST.....		$ 12,930

11. Method of Performance

The SSRL special facilities engineering design will be done by Laboratory (LBL, SSRL, and SLAC) personnel, as will major technical component construction and assembly. Technical component construction and fabrication will be done by a combination of SLAC shops and by subcontracts awarded on the basis of competitive bidding and managed by SSRL and SLAC personnel. Use of LBL shops will also be investigated for the fabrication of the SPEAR insertion device.

Conventional facilities engineering design will be performed under a negotiated Architect/Engineer subcontract. Inspection and some engineering will be done by Laboratory personnel. Construction and procurement will be accomplished by fixed-price subcontracts awarded on the basis of competitive bids.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	FY 1984	FY 1985	FY 1986	Total
a. Total facility construction costs:[a/]				
SSRL Enhancement[b/].....	$ 1,240	$ 8,630	$ 3,060	$ 12,930
Total facility construction cost.....	1,240	8,630	3,060	12,930

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Stanford Synchrotron Radiation Laboratory Enhancement
Stanford Linear Accelerator Center
Stanford, California

2. Project No.: 85-ER-402

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

b. Other project funding:	FY 1984	FY 1985	FY 1986	Total
SSRL R&D	700	700	0	1,400
Total R&D/Startup	700	700	0	1,400
Total Project Funding	$ 1,940	$ 9,330	$ 3,060	$ 14,330

a/ Includes escalation to midpoint of construction for all conventional facilities and compounded annually for special facilities; FY 1983 8%; FY 1984 8 1/2%; FY 1985 and beyond 9%.
b/ At the Stanford Linear Accelerator Center and includes the addition of an 18^{0} beamline.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding

(1) The major elements of the SSRL Enhancement have been described in Item 8. The funding profiles were determined as follows:

(a) At SSRL the PEP Beam Line will be accomplished during the first two years. Improvements to SPEAR are schedules for the second year and the Laboratory Office Building is scheduled for the second and third years. Completion of the SPEAR scattering Beam Line and the Light Assembly Shop will occur during the third year.

(2) Other project funding

(a) Insertion Devices and Beam Line Optical Elements R&D activities include superconducting wigglers, in-vacuum undulators, and advance beam line components suitable for ultra high brilliance photon beams.

(b) SSRL R&D is related in support of the construction project includes prototype development and R&D on technical components.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
BASIC ENERGY SCIENCES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Kansas State University, Ion Collision Physics Facility, Manhattan, Kansas

2. Project No.: 85-ER-403

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 2nd Qtr. FY 1985

4. Date construction ends: 4th Qtr. FY 1987

5. Previous cost estimate: None

6. Current cost estimate: $3,400

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1985	$ 3,400	$ 2,000	$ 2,000	$ 1,500
1986	0	1,400	1,400	1,000
1987	0	0	0	900

Financial schedule is based on the net Government funding associated with this project. The State of Kansas will provide an additional $600,000 for the conventional construction necessary to house the new capabilities.

8. Brief Physical Description of Project

The James R. MacDonald Laboratory will be expanded to house a new booster accelerator and a new low energy highly charged ion source. A 9,000 square foot basement addition will be required to house these facilities. The additional power requirement is 100 KVW. Very little additional water for cooling will be required.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Kansas State University, Ion Collision Physics Facility, Manhattan, Kansas

2. Project No.: 85-ER-403

8. Brief Physical Description of Project (continued)

New equipment to be installed in new basement addition includes:

A. Cryogenic ion source including electron gun, superconducting solenoid magnet. Analyzing magnet, accelerating column and beam line apparatus.

B. Superconducting linear accelerator includes resonators, amplifiers, power supplies, RF control system, superconducting solenoids, liquid nitrogen system, liquid helium refrigerator and storage dewar, accelerator control computer system, data acquisition and data reduction computer system.

9. Purpose, Justification of Need for, and Scope of Project

The construction of the ion collision physics facility, together with the existing atomic physics capability at Kansas State University, will constitute the Institute for Atomic Collision Physics. The project will involve construction and installation of (1) an advanced source of low energy highly charged ions of the CRYEBIS type and (2) a LINAC booster comprising twelve superconducting split-ring resonators. Each of these two additions will function as an adjunct to the existing tandem Van de Graaff in ways that, along with a dedicated system for high speed computation and data analysis, will have the capability to study the atomic physics of a spectrum of ions, energies and intensities unmatched in the world. This will open new areas of atomic collision physics, allow long beam time experiments, and provide a forefront environment for training young scientists and encouraging interdisciplinary cross-fertilization.

This project will be constructed on the Kansas State University campus, non-Government owned property.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Kansas State University, Ion Collision Physics Facility, Manhattan, Kansas

2. Project No.: 85-ER-403

10. Details of Cost Estimate

	Item Cost	Total Cost
a. Engineering, design and inspection		$ 100
b. Land and level rights		0
c. Construction costs		330
1) beam line construction	$ 315	
2) utilities	15	
3) buildings	*	
d. Equipment		2,370
e. Contingency		600
Total Project Cost		$ 3,400*

*Kansas State University will provide additional funding to construct the building. a) Estimate is based on completed conceptual design; b) Escalation is based on annual 8% to the mid-point of construction

11. Method of Performance

This type of construction is unique and therefore the conceptual design, final design, assembly, and testing will be done by the staff of Kansas State University. Component parts equipment and building construction will to the extent possible be based on fixed priced competitively obtained procurement actions.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1985	FY 1986	FY 1987	Total
a. Total project funding					
(1) Total facility costs					
(a) Construction line item	$ 0	$ 1,500	$ 1,000	$ 900	$ 3,400*
(b) CP&D	0	0	0	0	0
(c) Expense funded equipment	0	0	0	0	0
(d) Inventories	0	0	0	0	0
Total facility costs	$ 0	$ 1,500	$ 1,000	$ 900	$ 3,400*

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Kansas State University, Ion Collision Physics Facility, Manhattan, Kansas

2. Project No.: 85-ER-403

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

(2) Other project funding					
(a) R&D necessary to complete construction....	$ 0	$ 180	$ 180	$ 50	$ 410
(b) Other.....	0	0	0	0	0
Total other project funding.....	0	180	180	50	410
Total project funding.....	$ 0	$ 1,680	$ 1,180	$ 950	$ 3,810*

As noted above, the State of Kansas will provide an additional $600,000 for conventional construction of housing.

b. Related annual funding requirements (estimated life of project: 20 years)

(1) Operating costs.....	$ 0
(2) Programmatic operating expenses.....	600
(3) Capital equipment not related to construction but related to the programmatic effort in the facility.....	50
(4) GPP or other construction related to programmatic effort in the facility...	0
(5) Other costs.....	0
Total.....	$ 650

13. Narrative Explanation of Total Project Funding and Other Related Requirements

No narrative required.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
BASIC ENERGY SCIENCES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

3. Date A-E work initiated: 1st Qtr. FY 1984

3a. Date physical construction starts: 2nd Qtr., FY 1984

4. Date construction ends: 4th Qtr., FY 1986

5. Previous cost estimate:

6. Current cost estimate: $ 19,700
Less FY 1983 PE&D: 0
$ 19,700

Date: 9/83

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1984	$ 19,700	$ 2,500	$ 2,500	$ 2,200
1985	0	10,000	10,000	8,330
1986	0	7,200	7,200	9,170

Work included for accomplishment with the first year's appropriation of $2,500,000 will include but not be limited to the design and engineering of beam line components and preliminary and detail design of the support area construction.

8. Brief Physical Description of Project

Current program planning anticipates the need for the insertion devices (wigglers and undulators) and beam lines (front and end beam transport and experimental stations) to the existing VUV and X-ray rings. Design, fabrication and construction of up to three insertion devices and six beam lines is presently anticipated with the final configuration to be dictated by programmatic demands and the state of the art at the time of construction.

The project also provides for design and construction of building space to house technical work areas, laboratories and offices and provide additional experimental staging and support areas.

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

8. Brief Physical Description of Project (continued)

A. New Experimental Equipment

This project provides for an expansion of experimental capabilities which will be made available to general users from university, industrial, national and government laboratories. The greatest use is anticipated to be by materials scientists, but sizeable participation is expected by chemists, biologists and other disciplines.

The new equipment to be provided will take maximum advantage of the properties of the NSLS source. As noted above the exact design of this equipment will be determined as the project progresses to maintain the flexibility necessary to develop state of the art facilities which will ensure high quality research capabilities. Three beam lines and associated insertion devices have been designated. Up to three additional beam lines may be constructed as dictated by science and permitted by available resources.

1) High Q-Resolution X-Ray - This beam line and associated hybrid wiggler insertion device will provide high x-ray intensity levels for materials science research as well as biophysics and liquid crystal technology.

2) X-Ray Microscopy and Holography - This beam line and associated soft x-ray undulator insertion device will provide high brightness soft x-rays with photon energies from 0.28 KeV to 2.8 KeV to investigate three dimensional imaging. The technique will eliminate damage to specimens and allow simple sample preparation.

3) Superconducting Wiggler Line -his beam line will support high energy x-ray research in the field of digital subtraction imaging in medical systems without invasive chemical techniques. In addition the line will support a substantial materials research program.

B. New Building Addition

The proposed additions to the NSLS building will provide elementary support and staging areas, laboratories, technical work areas and offices to promote more effective utilization of the NSLS facility. The technical staff will move to new work areas, making more space available for the new beam lines. Extending the experimental space adjacent to portions of the VUV and X-ray storage rings will allow a number of long beam lines to be constructed, permit additional branching of existing ports, and give some extremely useful space to users for specialized support equipment.

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

8. Brief Physical Description of Project (continued)

The proposed building expansion consists of several additions to the existing facility. The largest of these will be approximately 21,000 square feet continguous to the x-ray floor area. The addition will contain a machine shop, angiography laboratory with separate ambulance entrance, general laboratories, darkrooms, offices, an experimental staging and support area, technical work area, mechanical equipment room, and several public rooms. A partial second floor of approximately 8,000 square feet will house NSLS staff and visiting research teams. A small addition to the west portion of the x-ray floor will provide three laboratories a study area and a staging area.

The VUV area will also have several additions providing beam line extension areas, experimental staging and support space, offices and a receiving area.

In order to provide the space necessary for the Light Source Staff located in satellite buildings a 7800 square foot 3rd floor will be added above the existing 2nd floor office wing of the NSLS building.

Several other additions including a tunnel connecting the new facility to technical work space in an adjacent facility, a lobby addition and covered walkway will be provided.

The expanded building will be designed to current DOE energy conservation standards and contain fire protection systems. Access by handicapped persons will be provided by extending the present elevator to the new third floor and a new elevator to the 2nd floor x-ray expansion.

C. Existing Facility

The NSLS consists of two electron storage rings, an injection system common to both, experimental beam lines, experimental equipment, and office and support area all of which is housed in a 74,000 square foot building.

The high energy x-ray storage ring provides for the possibility of 28 primary beam ports, each of which is capable of accommodating several experimental beam lines. The VUV ring provides for 16 beam ports which are also capable of accommodating several experiments each. In sum, more than 90 experiments can be carried out at one time when the facility is fully instrumented. In addition to general users, research groups called Participating Research Teams (PRT's) from universities, industry and national and government laboratories, upon advice by a program committee, and approval by the NSLS Department Chairman provide instruments to carry out research programs at the NSLS facility. Their instruments are made available to general users for 25% of the available time. At present such groups provide an additional 20 experiments at the facility. General users are able to use any of the experimental lines, PRT or community lines, upon approval of their experimental proposal.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

9. Purpose, Justification of Need for, and Scope of Project

The NSLS is operated as a user facility. This means that researchers from BNL and other laboratories will be able, after review of a proposal by a committee of distinguished scientists, and acceptance by the NSLS Department Chairman to carry out an experiment using either the UV or X-ray radiation produced by the rings.

The response from users, both within BNL and outside, has placed a demand on the NSLS facility far surpassing its present resources. The limited beam lines combined with the limited space available makes expansion of experimental research within the present confines of this facility unpracticable. In order to support further development of this facility it will be necessary to provide additional floor, laboratory, and staging space. An experimenter should have a choice of a wide range of instruments which he can utilize for this research. To provide this choice, two types of instruments are proposed:

a) A group of instruments that will be available to general users that will complement in capability those already provided, and;

b) Several instruments (wiggler magnets and an undulator) which will provide a range of wavelength and intensity not available at the bending magnets. These instruments will be used both by general users and by members of the Participating Research Teams who will require such capabilities for their experiments.

A. New Experimental Equipment

In the original development plan, provision was made for a total of eight beam lines to be available to general users. Additional beam lines were to be provided at the rate of about two a year out of capital funds. Further instrumentation was to be made available by Participating Research Teams (PRT's), who would install beam lines at the rings at their expense and who would make 25% of the experimental time on those lines available to general users. However, the growth in user participation has far exceeded earlier expectations.

In order to provide experimental capabilities required both by PRT's and by general users, it is proposed to accelerate beam line construction. It is particularly important that the capabilities provided for in this project, such as wiggler magnets, be made available at the earliest possible date.

In addition to satisfying the requirements of the users, the accelerated design and construction of these beam lines will provide a cost saving because of efficiencies in planning, design, and construction.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

9. Purpose, Justification of Need for, and Scope of Project (continued)

B. New Building

The design for the NSLS building emphasized long term space requirements for the accelerator/storage rings and the equipment associated with their control and operation. Adequate space for experimental beam lines around the VUV and X-ray storage rings was also provided, although future long beam lines that extended beyond the building walls were regarded as a possible future option.

The space for the machine and experiments was given highest priority in initial design, while support areas were provided to satisfy requirements for projected use during the initial years of operation. A possible expansion of experimental support areas, work areas, and offices was allowed as a future option. Therefore, only minimal space was given to several general laboratories, the second floor office-administration area, and other support areas.

It was projected that during the early years of operations, up to approximately 50% of the 28 X-ray and 16 UV ports would be utilized. The extremely enthusiastic response of the scientific community now forces us to advance the expected rate of beam line construction and building expansion. More than 20 experimental have been proposed by PRT's, which are expected to be constructed at an early date. This response, coupled with the beam lines to provide by the project, indicate that the experimental floor will be extremely crowded beyond October 1983 and additional support space will be essential.

The original design anticipated a possible need for future expansion. The building frame was designed to support a third floor over the office administration wing. Site utility lines were kept at least 30 feet from the building foundation. Adequate space was left between the NSLS buildings and the Safety and Environmental protection building.

In addition to the pressing need to return experimental floor space to its intended use, the expansion will provide adequate office space for the permanent staff and work areas to complement the research and development associated with the anticipated experimental and machine improvement programs. The short connecting tunnel between the NSLS building and the basement of the adjacent Instrumentation building will connect the NSLS staging areas to an area where now extensive NSLS vacuum, instrument, and diagnostic work is in progress and where UV and X-ray test sources are located.

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

9. Purpose, Justification of Need for, and Scope of Project (continued)

Annual Costs

The estimated incremental operating costs of the proposed NSLS beam lines and support area construction are listed below. Costs are in the FY 1984 dollars.

	(Dollars in Thousands)
Materials, Supplies, Support Services	$ 95
Electric Power	178
General and Administrative	42
Total	$315

10. Detail of Cost Estimate[a/b/]

	Item Cost	Total Cost
a. Engineering, design and inspection, including A-E fee (approx. 21% of item c)..	$	$ 2,970
b. Land and land rights.....		0
c. Construction costs.....		13,335
(1) Beam line construction.....	6,030	
(2) Improvements to land.....	110	
(3) Building.....	6,925	
(4) Tunnel to S&EP building.....	90	
(5) Utilities.....	180	
d. Standard equipment.....		800
Subtotal.....		17,105
e. Contingency, approximately 17% of above costs.....		2,595
Total Project Cost.....		$ 19,700

a/ Estimate is based on a complete conceptual design.

b/ Escalation rates conform to the guidelines prescribed in the Department of Energy Field Budget Process Chapter, February 1983, which are based on the materials and labor data contained in the Energy Supply Planning Model and escalation rates forecasted by Data Resources, Incorporated (DRI). Current costs have been escalated by 7.6%, 8.6% and 8.7% per year for FY 1984 through FY 1986.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

11. Method of Performance

Insertion device and beamline construction is unique and therefore the conceptual design, final design, assembly and testing will be done by the staff of the National Synchrotron Light Source of the Brookhaven National Laboratory. Component parts wherever possible will be fabricated by industry under fixed priced competitively obtained procurement actions. Some components may be fabricated in the existing shops at BNL. It is also anticipated that other laboratories, private consultants, and industrial firms will be used for advice on specific problems. Building design will be on the basis of a negotiated architect-engineer contract and its construction will be by a competitively obtained lump sum contract which may be phased.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1984	FY 1985	FY 1986	Total
a. Total project costs					
1. Total facility costs					
(a) Construction line item.....	$ 0	$ 2,200	$ 8,330	$ 9,170	$ 19,700
(b) CP&D.....	0	0	0	0	0
(c) Expense Funded Equipment.....	0	0	0	0	0
(d) Inventories.....	0	0	100	100	200
Total facility costs.....	0	2,200	8,430	9,270	19,900
2. Other project costs					
(a) R&D necessary to complete construction of beam lines....	900	500	500	0	1,900
(b) Other.....	0	0	0	0	0
Total other project funding....	900	500	500	0	1,900
Total project funding.....	$ 900	$ 2,700	$ 8,930	$ 9,270	$ 21,800

1. Title and location of project: Beam lines and support area construction
National Synchrotron Light Source (NSLS)
Brookhaven National Laboratory, Upton, NY

2. Project No.: 84-ER-111

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

b. Total related funding requirement (estimated life of project: 17 years)

1. Operating costs	$ 288
2. Programmatic operating expenses directly related to the facility	0
3. Capital equipment not related to construction but related to the programmatic effort	0
4. GPP or other construction related to the programmatic effort	0
5. Other costs	0
Total other related annual funding requirements	$ 288

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
   1. Total Facility
      (a) Construction line item - no narrative required.
      (b) CP&D - no narrative required.
      (c) Expense funded equipment - no narrative required.
      (d) Inventories - it is anticipated that funds will be required for the procurement of special process spares.
   2. Other project funding
      (a) R&D necessary to complete construction - funds provided in the NSLS R&D budget. This item gives estimates of the R&D necessary to develop the monochromators, mirror systems, target chambers, detectors and superconducting structures for high field wigglers and undulators.
      (b) Other - no narrative required.

b. Total related funding requirements
   1. Operating Costs - There will be an annual requirement of additional materials, supplies, and support services associated with the new beam lines. Also, there will be a requirement for increased facility electrical power.
   2. Programmatic operating expenses directly related to the facility - no narrative required.
   3. Capital equipment not related to construction but related to the programmatic effort - no narrative required.
   4. GPP or other construction related to the programmatic effort - no narrative required.
   5. Other costs - no narrative required.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
BASIC ENERGY SCIENCES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Center for Advanced Materials, Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

3. Date A-E work initiated: 2nd Qtr. FY 1984

3a. Date physical construction starts: 2nd Qtr. FY 1984

4. Date construction ends: 4th Qtr. FY 1988

5. Previous cost estimate: $138,900

6. Current cost estimate: $ 40,250
Less FY 1983 PE&D: 0
$ 40,250
Date: 8/83

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1984	$ 1,760	$ 1,760	$ 1,760	$ 1,760
1985	38,490	10,790	10,790	10,290
1986	0	14,440	14,440	12,940
1987	0	13,260	13,260	14,000
1988	0	0	0	1,260

8. Brief Physical Description of Project

The Center for Advanced Materials (CAM) is comprised of two research laboratories. This is a continuation of the FY 1984 request, Center for Advanced Materials (CAM), and which takes into consideration the recommendations of the ad hoc review Panel.

The Research Laboratories will involve two new laboratory complexes at LBL, the Surface Science and Catalysis Laboratory (SSCL) and the Advanced Materials Laboratory (AML).

1. Title and location of project: Center for Advanced Materials
Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

8. Brief Physical Description of Project (continued)

The CAM facilities at LBL will be located on University of California property adjacent to the Berkeley campus, within the site of the Lawrence Berkeley Laboratory. The project will include the construction of new facilities, and the alteration of, and additions to, existing facilities. Plant and site facilities will consist of: a) improvements to land, including grading, drainage, paving, lighting, and walkways; b) a new Surface Science and Catalysis Laboratory (SSCL) building (47,500 GSF), located near the existing Materials and Molecular Sciences Laboratory (Building 62); c) the new 82,000 GSF building, the Advanced Materials Laboratory (AML); d) the extension of existing utilities, including electrical power, water, sewage, gas, and communications; and e) standard equipment and special facilities including office and laboratory furniture and equipment, fume hoods, ventilation and temperature control equipment, laboratory diagnostics and instrumentation equipment, fire protection equipment and computation equipment.

Conventional Construction

The Surface Science and Catalysis Laboratory will be located near the existing Materials and Molecular Sciences Laboratory (Building 62). The 3-story building will have a reinforced-concrete frame, shear walls, waffle roof-and-floor structure supported on spread footings. Auditorium and administrative area roofs will utilize metal deck on steel framing. The floor plan is approximately 95 x 150 feet.

The Advanced Materials Laboratory will consist of a single light-laboratory building. The proposed four-story building will occupy a hillside site providing a first floor with a main entrance at the grade level of the base of the hill. The full floor-plan will be L-shaped, about 192 feet long in one direction and 173 feet in the other; the longer element will be 63 feet wide and the other, 96 feet wide. The building structure will consist of a reinforced concrete frame with shear walls. Roof and floors above the base level will be of waffle-slab construction. Foundations will consist of poured-in-place reinforced concrete caissons.

Finishes on the new buildings will include: standard built-up roofing over insulation; exterior (non-bearing) walls of prefinished panels on metal studs (insulated cavity); and gypsum board interior wall surfaces throughout. Acoustical ceilings will be needed in certain areas; otherwise ceilings will be painted gypsum board. Laboratory furniture and fume hoods will be commercial products with acid/alkali-resistant tops and construction. Building elevators will be rated for 6000 lb. capacity, suitable for carrying freight and passengers. Heating ventilating and air conditioning (HVAC) needs will be met by central station air-handling units, draw-through cooling coils, return fan units and economizer controls. All supply and return air will be ducted. All buildings will be equipped with automatic fire springler and alarm systems. Utilities will be extended from nearby existing plant services.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Center for Advanced Materials
Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

9. Purpose, Justification of Need for, and Scope of Project

This research center is being proposed as a major scientific redirection of the Lawrence Berkeley Laboratory to address a vital national need, to accelerate basic research in an area that promises medium-term impact on high-technology industries, and to foster closer ties between national laboratory researchers and their counterparts in industrial and university laboratories. The CAM project will have two major objectives:

- To enhance understanding, through long-range basic research, of the synthesis, characterization, and properties of advanced materials in support of U.S. energy-related and high-technology industry.
- To provide advanced facilities for research training of additional graduate students in physical sciences and engineering fields vital to U.S. high-technology industry.

For three decades following the end of World War II, the United States led the world in materials research. In the last few years, we have been approached and sometimes passed in critical high-technology industries by Japanese and German companies, notably in such production areas as electronics, microcircuits, and specialty steels. One important reason for this deteriorating situation is that our foreign competition has produced reliable materials and parts for advanced technological applications. Their success, which reflects improved control of compositions and structures at every stage from powder or ingot to finished device, was made possible by coordinated research on the materials themselves and on sophisticated devices for materials characterization and automated processing control.

The West German and Japanese governments are supporting massive research programs to further their aggressive high-technology industrial development. For this country to mount a comparable interdisciplinary attack on the materials and materials-processing problems requires input from basic research efforts with longer time scales and higher risk than can reasonably undertaken by U.S. companies. The research needed also requires investments in improved apparatus and instrumentation that will strain the present resources of publicly-supported materials laboratories in this country.

The CAM project will provide the modern tools and facilities required for making possible major advances in energy-related and high-technology industries by improving the scientific understanding of the underlying chemical and physical phenomena that influence both materials and device behavior.

1. Title and location of project: Center for Advanced Materials
Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

9. Purpose, Justification of Need for, and Scope of Project (continued)

Research Laboratories

Two research laboratories form the major components of the CAM:

- The Surface Science and Catalysis Laboratory (SSCL). A laboratory devoted to surface and catalysis studies using state-of-the-art instrumentation techniques.
- The Advanced Materials Laboratory (AML). A laboratory devoted to interdisciplinary study of the synthesis and characterization of energy-related, high-technology, and strategic materials. In addition, there will be research on the design of high-technology devices utilizing new materials and the design of innovative devices for the characterization of materials-property relationships.

Both the SSCL and the AML will be based on strong programs that already exist at LBL. Other elements are completely new, but they too build on experience and personnel already at LBL and at the adjacent University of California Berkeley campus. The first CAM research program associated with the above will be initiated in FY 1984.

Because of the pressing need to retain high-technology leadership, the proposed project schedule calls for the start of construction in FY 1984 and the completion of all facilities in FY 1988. Delays would extend the time at which research results can be generated and transferred to U.S. industry. A CAM Advisory Board composed of scientific leaders from industry, universities, and Federal laboratories will advise the LBL director on CAM scientific program directions to ensure that CAM basic research addresses America's long-range high-technology needs. The CAM affiliates, consisting of major research teams from industry and universities, will participate in CAM. The following cost estimates and mix among facilities may vary depending upon the research and development progress, but does represent the current plan.

This project will be constructed at the Lawrence Berkeley Laboratory which is non-Government owned property.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Center for Advanced Materials
Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

10. Details of Cost Estimate

a. Engineering, design, inspection and administration	4,220
b. Construction costs	23,280
c. Standard equipment	6,350
d. Removals and relocations	360
e. Contingencies at approximately 15% of above	6,040
TOTAL ESTIMATED COST	$40,250

11. Method of Performance

Conventional facilities engineering design will be performed under a negotiated Architect/Engineer subcontract. Inspection and some engineering will be done by Laboratory personnel. Construction and procurement will be accomplished by fixed-price subcontracts awarded on the basis of competitive bids.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	Total
a. Total facility construction costs:[a/]						
SSCL	$ 1,760	$ 8,690	$ 1,500	$ 0	$ 0	$11,950
AML	0	1,600	11,440	14,000	1,260	28,300
Total facility construction cost	1,760	10,290	12,940	14,000	1,260	40,250
Total Project Funding	$ 1,760	$10,290	$12,940	$14,000	$ 1,260	$40,250

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Center for Advanced Materials
Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

Other related funding requirements (estimated life of project: 25 years)

	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
Programmatic research	$ 2,300	$ 3,300	$ 7,800	$11,300	$11,300	$11,300
Capital equipment related to programmatic research	1,300	1,650	1,900	2,700	2,700	2,700
Total	$ 3,600	$ 4,950	$ 9,700	$14,000	$14,000	$14,000

*/ Includes escalation to midpoint of construction for all conventional facilities and compounded annually for special facilities; FY 1983 8%; FY 1984 8 1/2%; FY 1985 and beyond 9%.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding

(1) The major elements of the CAM facility have been described in Item 8. The funding profiles were determined as follows:

(a) The Surface Science and Catalysis Laboratory has a completed Title II design. Construction will be packaged with site preparation scheduled for FY 1984 so that building construction can be completed in the fourth quarter of FY 1986.

(b) The Advanced Materials Laboratory building is scheduled for Title I review in the first quarter of FY 1985. The project will be scheduled to sequence bid packages to minimize disruption to existing programs and construction congestion and to optimize favorable bidding conditions and work leveling. Site bid packages will be let in the third quarter of FY 1985 and in the first quarter of FY 1986. Building construction will begin in the second quarter of FY 1986 and end in the fourth quarter of FY 1988.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Center for Advanced Materials
Lawrence Berkeley Laboratory, Berkeley, California

2. Project No.: 84-ER-112

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements (continued)

b. Other related funding requirements

The annual costs of the scientific program are increased progressively to build up a high quality research staff for the CAM laboratories. Funding in the early years of the project is mainly to attract superior senior scientists to lead the new scientific programs described in Item 9. These researchers can be housed initially on the University campus and then in the SSCL Building until all conventional facilities are completed. The programs will expand in the latter years of the project to include the full complement of scientists and technicians. The capital equipment needs related to this research staff buildup reflect Laboratory experience that numerous laboratory equipment items will be needed at the level of approximately 20% of the operating program budget. These amounts were augmented in the first two years to take into account startup capital equipment needs.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
LEAD TABLE
ENERGY RESEARCH ANALYSIS
SUPPORTING RESEARCH AND TECHNICAL ANALYSIS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
(Tabular dollars in thousands. Narrative material in whole dollars)

	1983 Appropriation	1984 Appropriation	1985 Base	1985 Request
Energy Research Analysis				
Operating Expenses.....	$ 2,819	$ 2,869	$ 2,869	$ 3,000

Authorization: Section 209, P.L. 95-91.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
SUMMARY OF CHANGES
ENERGY RESEARCH ANALYSIS
(In thousands of dollars)

1984 Appropriation enacted.....	$ 2,869
o Cost of living increase.....	+ 131
1985 budget request.....	$ 3,000

The Energy Research Analysis program is aimed at providing DOE with the capability for independent, objective analysis of the Department's technical needs and opportunities. Its current objective includes (1) assessing the adequacy of the technology base supporting R&D programs; (2) performing independent analyses and technology assessments of R&D programs; (3) providing coordination and direction in interagency activities such as acid rain ($600,000); (4) developing issues and alternative actions to support policy decisions; and (5) providing support to Departmental advisory groups such as the Energy Research Advisory Board (ERAB). These activities are carried on through studies, workshops, panels and other mechanisms which permit the Department to make use of the best available scientific and technical talent both inhouse and from industry and academia. Projects are identified through staff analysis, contact with other DOE program staff, contact with outside experts and through the various R&D program planning functions of the Department.

Recent Accomplishment

- Recent assessments of the adequacy of DOE's technology base included the review by the Fossil Energy Research Working Group (FERWG), an industry, academic and Government work group, who defined R&D needs in shale oil, tar sands and heavy oils.
- Program analysis completed during FY 1983-1984 were:
  - Two major program assessments (university and laboratory research projects in Fossil Energy's Enhanced Gas and Oil Recovery Program and Health and Environmental Research programs);
  - Reviews of research objectives that led to a reexamination of program emphasis, e.g., MHD.
  - An assessment by JASON, a group of physicists who are expert consultants to DOD, who concluded a review of "Heavy Ion Fusion."
- Recent and anticipated issue and alternative action studies were:
  - Issue papers prepared for the Under Secretary
  - Assisting in international representation of U.S. Energy R&D policies (to the IEA).
- Recent Departmental coordination responsibilities included the subjects of:
  - Acid Rain, through participation in Interagency Task Forces (Transboundary Air Pollution Coordinating Committee & Interagency Task Force on Acid Precipitation). Coordinating all DOE action on acid rain research and providing input to Interagency Task Forces activities.
  - Strategic Minerals, through participation in the efforts of the Interagency Working Group in Strategic Minerals Policy.
  - Satellite Imagery, through participation in the Interagency Program Board on Civil Operational Land Remote Sensing from Space.
- Support of the assessments and advice provided by groups, such as the Energy Research Advisory Board (ERAB), to the Secretary, DOE.

Projected Activities

- Technology Assessments:
  - Up to four assessments of technologies (such as shale beneficiation or nuclear waste) each year depending on complexity and depth.
  - Up to four program assessments to determine research needs and status of technology (such as Solar, Wind, Geothermal, Photovoltaics or Waste Management).

- o Analyses of Research:
  - Comparison analyses of the recommendations of advisory groups versus actual research programs (such as Fossil Energy Basic and Applied Research).
  - Reviews of research that crosscut Departmental programs for integration of objectives and direction approaches (such as acid precipitation).
- o Provide technical coordination and guidance:
  - Maintain Departmental coordination for Acid Precipitation, Strategic Minerals, Civil Land Remote Sensing.
  - Support the Director, Office of Energy Research, on reassessments of the Department's R&D priorities, programs and technology base.
- o Provide independent peer review of technical or research subjects directed by principal Secretarial Offices or the Director, Office of Energy Research.
  - The Coal Combustion Research Working Group, an industry, academic and Government group, will define research needs in coal combustion by early FY 1984.
  - Other groups formed for specific review tasks such as Gas and Oil Recovery and Large Scale Systems.
- o Advisory groups, such as ERAB, will be supported for the Department at the direction of the Secretary.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
LEAD TABLE
UNIVERSITY RESEARCH SUPPORT
SUPPORTING RESEARCH AND TECHNICAL ASSISTANCE
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
(Tabular dollars in thousands. Narrative material in whole units)

	1983 Appropriation	1984 Appropriation	1985 Base	1985 Request
University Research Support (ER)				
Operating Expenses:				
University/National Laboratory Cooperative Research				
University Laboratory Cooperative Research	$ 4,284	$ 3,500	$ 3,500	$ 6,550
University Reactor Fuel Assistance	1,704	1,500	1,500	1,900
Subtotal	5,988	5,000	5,000	8,450
Energy Manpower Development				
Energy Manpower Assessment	0	270	270	450
Energy Education and Training	0	200	200	300
Subtotal	0	470	470	750
Total				
Operating Expenses	5,988	5,470	5,470	9,200
University Research Support	$ 5,988	$ 5,470	$ 5,470	$ 9,200

Staffing FTE Requirements included in "Advisory and Oversight Program Direction" decision unit.

Authorization: Section 209, P.L. 95-91, Section 31, Atomic Energy Act of 1954, Section 103(10), P.L. 93-483

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL REQUEST
SUMMARY OF CHANGES
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
UNIVERSITY RESEARCH SUPPORT
(In thousands of dollars)

1984 Appropriation enacted	$ 5,470
1985 base	5,470
Program increases and decreases:	
University/National Laboratory Cooperative Research	
o Supports approximately 50 percent more faculty and student research and special training appointments at the Department's national laboratories, including institutes and workshops for high school science and math teachers	+ 3,050
o Provides fuel for two additional university nuclear research/training reactors, five additional reactor sharing projects and safety studies on the conversion of research reactors with high-enriched uranium fuel for the use of low-enriched fuel	+ 400
Subtotal	+ 3,450
Energy Manpower Development	
o Increases coverage of energy manpower supply/demand studies	+ 180
o Supports additional Prefreshman Engineering Projects for minority/women high school students	+ 100
Subtotal	+ 280
1985 budget request	$ 9,200

The principal goal of the University Research Support (URS) program is to help maintain strong scientific/technical research capabilities in support of the Department's long range energy R&D mission in both the university community and the national laboratories. This is accomplished through specialized research and manpower development efforts which complement and support the R&D mission of other Departmental programs. The URS program provides a Departmental focus for several efforts which involve universities both directly or in conjunction with the Department's national laboratories and major contractors. Individual efforts carried out through the URS program must relate to one or more of the following mission objectives:

- o Maintain and strengthen university-based energy research and manpower development efforts in selected high priority energy research fields.
- o Utilize the unique resources of the national laboratories (equipment, instrumentation, and personnel) for university faculty and student research and training.
- o Increase the number and enhance the quality of students including women and minorities pursuing professional level degrees in energy-related science or engineering.
- o Help strengthen the scientific/technical workforce in the Department's national laboratories.

URS supported activities may be distinguished from other Department programs by their multidisciplinary nature and by their focus on manpower/development needs and requirements for long range research.

The URS program consists of two major subprograms. The first subprogram, University/National Laboratory Cooperative Research, is directed at strengthening the capabilities of both universities and national laboratories as major energy research performers in the conduct of long range energy research. Many of the activities supported within this subprogram involve joint efforts between university and laboratory-based researchers. The second subprogram, Energy Manpower Development, includes efforts to increase the number of students pursuing energy-related engineering and science careers. This subprogram also includes support for implementing the Department's statutory responsibility for assessing the supply and demand of manpower for both current and projected energy R&D programs.

In order to carry out URS program objectives, a variety of approaches are used including university faculty research appointments, graduate and undergraduate research participation in national laboratory programs, joint efforts involving laboratory and university scientists and support for the operation of unique university-based nuclear research and training reactors.

In FY 1984, the following major accomplishments are planned for the URS program.

- o Support 1900 faculty and student participants in Lab/Coop activities at Departmental laboratories and contractor facilities.
- o Ensure the continued availability of fuel for university research reactors. (The Babcock and Wilcox Co. in Lynchburg, Virginia, is the sole U.S. supplier of plate-type fuel for DOE and university research reactors.) Continue reactor "sharing" projects at 16-18 universities for faculty and students from over 100 neighboring colleges and universities that do not have direct access to such research facilities.
- o Complete administrative support of 57 graduate research traineeships in four engineering disciplines (each graduate student is involved in a dissertation research project of direct interest to either industry or a DOE national laboratory).

- Continue the analysis of the supply/demand for manpower in energy R&D programs including preparation of the second comprehensive overview manpower information study in a number of energy R&D areas of direct relevance to the Department.

- Support approaches designed to strengthen the relationships between the national laboratories and minority universities including the support of joint research and manpower development efforts involving the Lawrence Berkeley Laboratory with Jackson State University, and the Argonne National Laboratory with Atlanta University.

- Support 15 Prefreshman Engineering Program projects which will maintain the opportunity for minority and disadvantaged high school students to select careers in science and engineering. Also includes support for five projects at DOE laboratories to provide special training, including "hands-on" research opportunities, to approximately 155 high school science teachers in such areas as energy resource studies, physics, chemistry and computer science.

	FY 1983	FY 1984	FY 1985 Request
University Research Support.....	$ 5,988	$ 5,470	$ 9,200

The FY 1985 request for the University Research Support Program is $9,200,000, an increase of $3,730,000 over the amount available in FY 1984. The principal priorities at the requested budget level are as follows:

- Supports approximately 3000 student and faculty research participation appointments and special training activities at the Department's national laboratories and major contractor facilities.

- Refuel up to six university research/training reactors and supports approximately 18 reactor sharing projects.

- Update manpower assessments for future professional level (scientists/engineers) manpower requirements for Departmental research programs.

- Supports cooperative projects with universities, industry and the Department's national laboratories through the PREP Program which is designed to encourage secondary school students to pursue energy-related engineering and science programs during their college careers.

- Supports six to eight high school science and math teacher institutes in computer science and energy-research related subjects at the DOE national laboratories.

The following sections describe the proposed activities which will be carried out at the FY 1985 Request level within each of the major URS subprograms.

University/National Laboratory Cooperative Research..	$ 5,988	$ 5,000	$ 8,450

The FY 1985 request for the University/National Laboratory Cooperative Research subprogram is $8,450,000, an increase of $3,450,000 over the amount available in FY 1984. The major goal of this subprogram is to strengthen research and manpower development-related efforts involving both the national laboratories and universities.

University-Laboratory Cooperative Research.....	($ 4,284)	($ 3,500)	($ 6,550)

The Administration and the Department are placing strong emphasis on strengthening the interrelationships between the national laboratories and the industrial and university sectors. The University-Laboratory Cooperative Research activity is an essential part of this overall emphasis and significant increases are proposed for FY 1985 for all categories of support within this area.

This activity includes a number of efforts ranging from precollege education, undergraduate and graduate student research; to faculty and postdoctoral level research participation and training at the Department's national laboratories and other contractor facilities. The principle goal of this program is to use the unique facilities and resources of the national laboratories to assist in the process of training and preparing university faculty and students for participation in future energy R&D programs. These activities also provide the Department's laboratories with additional research capabilities through participating faculty and their universities.

This program is administered by taking advantage of the diversified research facilities and resources of the Department's national laboratories and contractor network. Support is provided to ten multiprogram laboratories and related university consortia (who interact with 50 Departmental facilities) for the placement of faculty, postgraduate, graduate and undergraduate students in summer or academic year research and training programs and to assist in the development of cooperative research programs involving laboratory and university scientists.

The FY 1985 request includes support for the following:

- Undergraduate Student Research: The number of undergraduate science and engineering students supported in research assignments in participating laboratories will be increased by 50 percent over prior years. Each student will be assigned to an ongoing laboratory research program and will be involved in "hands on" energy research. Efforts will be made to continue to attract undergraduate students in engineering and science who are in the top 10 percent scholastically in their respective colleges. A related purpose of these efforts will be to encourage the best undergraduate students to pursue graduate work in an energy-related engineering or scientific field.

- Secondary School Teachers: Special workshops and institutes will be conducted at several DOE laboratories in FY 1984 designed to strengthen high school curricula and teaching skills in such key energy-related areas as physics, chemistry, and computer science. Several laboratories already have had experiences in carrying out 5-day workshops and evening and Saturday sessions throughout the year for high school science and math teachers in their areas. In 1985, primary emphasis will be placed on directly involving working level scientists in assisting high school teachers and students.

- Graduate Student Research: Graduate students thesis research support will be increased by 50 percent at participating DOE laboratories. Particular emphasis in 1985 is placed on involving these graduate students with ongoing research at the laboratory and maintaining close coordination with the student's faculty advisor back on campus.

- Faculty Research: One of the most productive periods of exchange between a university faculty member and laboratory staff occurs when the assignment covers a lengthy period of joint research or interaction. A sabbatical leave provides such an opportunity. Due to the dual benefits to the university and to the laboratory, in FY 1985 an effort will be made with the sponsoring DOE research programs to jointly support at least 30 university sabbatical assignments. Faculty research appointments for summer and academic year research will be increased by 30 percent over FY 1984 and will include cost sharing.

- Special Energy R&D Training: College faculty and student participants will continue to be supported in FY 1985 in special energy-related workshops, short courses, and institutes held at the national laboratories on selected topics at the forefront of energy R&D. Topics covered in past workshops include breeder reactor technology, transmission electron microscopy and chromatographic analysis of energy-related pollutants.

	FY 1983	FY 1984	FY 1985 Request
University Reactor Fuel Assistance	($ 1,704)	($ 1,500)	($ 1,900)

The objective of this activity is to provide fuel for university research reactor facilities with Materials Test Reactor (MTR) type fuel elements. The university-based nuclear research and manpower development effort is highly dependent on these specialized research and training reactor facilities. These dual purpose reactors are used both as a source of neutrons for research in the basic sciences as well as for graduate training in nuclear engineering. Fuel for the reactors is fabricated under a contract with the Department and "loaned" to the universities for use in the reactors. Additional support is provided to help defray reactor operational costs when the reactor is "shared" with researchers at neighboring universities. Support from this activity ensures that a continuing fuel supply is available for the operation of university research reactors which in turn are essential national facilities for the preparation and training of professional level manpower for the nuclear industry. As a result of the Nuclear Non-Proliferation Act of 1978, DOE is developing the fuel technology for the replacement of high enriched fuel with low enriched uranium. The conversion of selected domestic university research reactors was initiated in FY 1984.

At the FY 1985 request level, up to 6 reactors will be refueled during FY 1985 and approximately 18 reactor sharing grants will be made on a competitive basis. In addition a comprehensive cost assessment will be completed on the budget impact of converting each university research reactors serviced to low enriched uranium.

Energy Manpower Development	$ 0	$ 470	$ 750

The FY 1985 request for the Energy Manpower Development subprogram is $750,000, an increase of $280,000 over the amount available in FY 1984. This subprogram combines two manpower-oriented efforts -- Manpower Assessment conducts studies and analyses of the supply and demand of manpower for both current and future energy R&D programs, and the Energy Education and Training effort supports activities directed at encouraging secondary school students to pursue energy-related science and engineering programs at the college level.

Energy Manpower Assessment	($ 0)	($ 270)	($ 450)

Under Section 103 (10) of the Energy Reorganization Act of 1974 the Department is required to assure "the collection, analysis, and dissemination of necessary manpower supply and demand data" to carry out energy-related programs. In responding to this mandate, the Manpower Assessment effort, in conjunction with other Federal agencies, develops and maintains information systems to provide both governmental and private sector managers with current and projected data on the supply and demand of energy-related scientific, engineering and technical manpower, at all occupational and degree levels, disaggregated to national, regional and state areas.

In FY 1984, Manpower Assessment activities included completing an analysis of the effect of changing energy R&D funding and production activities on the employment and utilization of scientists, engineers, and related manpower working in energy. This activity (in cooperation with NSF) also continued its assessment of the participation of recent science and engineering graduates at all degree levels in energy-related programs. A new survey of nuclear occupational employment covering private industry and DOE contractor operated laboratories and facilities was also completed. This data provides DOE nuclear program managers, the NRC, private nuclear energy planners, and educational institutions with current and trend data on changing occupational profiles resulting from shifting emphasis among various nuclear activities.

The FY 1985 budget request of $450,000 will ensure the continuation of the collection, analysis and dissemination of baseline-type data on the employment and utilization of scientists and engineers in developing varied energy sources and programs. This effort will require sample surveys (in conjunction with NSF annual surveys) of doctoral scientists and engineers in energy R&D and other related programs, and new science and engineering graduates entering the labor market primarily involved in energy-related activities. Support will also be provided for the continuation of two projects related to nuclear technology developments: the biennial survey of occupational employment in nuclear-related activities in private industry and government owned-contractor operated facilities, and the continuing study and analysis of the current and potential supply of new nuclear engineering and health physics/radiation protection graduates needed for research, operations, and health, and safety activities.

The requested funding level will also enable this activity to support several additional projects particularly useful to policy decision makers and planners both in government and the private sector. These include: (a) an indepth assessment of manpower supply and demand for selected segments of the nuclear industry; (b) studies relating to the changing patterns of scientific and technical staffing and mobility in the Department's laboratories; and (c) biannual "quick response" surveys of the current supply/demand market for scientific, engineering, and technical specialties in selected energy industries.

	FY 1983	FY 1984	FY 1985 Request
Energy Education and Training.....	($ 0)	($ 200)	($ 300)

The Department of Energy plans an important supporting role in the area of science and math education in secondary schools, both through the support of secondary school teacher and student training projects sponsored by the Department's national laboratories and through continuing to support Prefreshman Engineering Program projects (PREP) in FY 1985. Under this activity, competitive grants are awarded to engineering schools to select junior and senior high school, minority and women students to participate in summer enrichment activities. These activities range from science and math courses, computer programming, energy-related engineering exercises, field trips to engineering industries, etc. Successful engineers serve as role models for the participants. Local industry provides substantial matching support for this effort. Evaluative studies show that over two thirds of the PREP participants pursue engineering or other science course offerings in college. Finally, as in prior years, support will be provided for energy-related student research projects at the International Science and Engineering Fair and similar competitions.

At the FY 1985 request level a total of 20 PREP projects would be funded, reaching over 2,000 students.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
LEAD TABLE
UNIVERSITY RESEARCH INSTRUMENTATION
SUPPORTING RESEARCH AND TECHNICAL ANALYSIS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
(Tabular dollars in thousands. Narrative material in whole dollars)

	1983 Appropriation	1984 Appropriation	1985 Base	1985 Request
University Research Instrumentation (ER) Operating Expenses	$ 0	$ 4,000	$ 4,000	$ 6,000
Total Operating Expenses University Research Instrumentation	0	4,000	4,000	6,000
	$ 0	$ 4,000	$ 4,000	$ 6,000

Authorization: Section 209, P.L. 95-91

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL REQUEST
SUMMARY OF CHANGES
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
UNIVERSITY RESEARCH INSTRUMENTATION
(dollars in thousands)

1984 Appropriation enacted	$ 4,000
1985 base	4,000
Program increases and decreases:	
University Research Instrumentation	
o Provides support for additional Research Instrumentation awards	+ 2,000
1985 budget request	$ 6,000

The University Research Instrumentation Program provides support to university research groups on a competitive basis for the purchase of major, state-of-the-art scientific research instrumentation which is essential for continued progress in advanced energy-related scientific and technical research.

The continued improvement of energy technology is dependent upon the availability of new knowledge and concepts which are applicable to energy-related materials and processes. For example, improving catalytic processes or the efficiency of photoconductors requires increased understanding of electron transfer or the occurrence of intermediate reactions which occur at or near the surfaces of such materials. However, the rapidity with which these reactions occur and the short lifetimes of the intermediate products make it difficult to detect what has occurred unless one uses very sophisticated instrumentation, including dedicated computers which make it possible to obtain, store and analyze the large volume of data which often is required.

The types of instruments required for advanced energy research include plasma emission spectrometers which can detect and identify materials at the parts per billion level, a variety of scanning microscopes which can be used to obtain greater understanding of surface states and features, and hydrothermal equipment which enables one to simulate the temperatures and pressures which are found deep within the earth and in ocean depths. These and related instruments are very expensive, generally of the order of several hundred thousand dollars, and thus beyond the means of nearly all research universities to finance directly.

In recent years the Department has attempted to aid universities to obtain access to these and similar sophisticated research instruments by (1) making the equipment at its national laboratories available to university researchers, (2) establishing unique user-oriented research facilities in areas such as combustion research and (3) providing some funds for the less expensive research tools required in conjunction with its research projects. None of these programs, however, meets the need for the continuous availability on campus of the type of equipment which is provided through this program.

In FY 1984 the Department, in cooperation with several other Federal agencies including DOD and NSF, initiated a University Research Instrumentation Program in an effort to help reduce the shortage of the state-of-the-art research instrumentation in the nation's major universities. This interagency effort is coordinated by the Interagency Working Group on Research Instrumentation chaired by the Deputy Director of the National Science Foundation and reporting to the Director of the Office of Science and Technology Policy. The principal objective of DOE's program is to improve the effectiveness of long-range research by helping universities to increase their capabilities to undertake advanced research in the most important energy R&D areas of concern to the Department's basic and technology programs. Instrumentation assistance will be provided on a competitive basis to approximately 10-15 universities.

	FY 1983	FY 1984	FY 1985 Request
University Research Instrumentation.....	$ 0	$ 4,000	$ 6,000

The FY 1985 Request for University Research Instrumentation Program is $6,000,000, an increase of $2,000,000 over FY 1984.

DOE's University Research Instrumentation Program will concentrate on those university groups which have already demonstrated expertise in one one or more of a small number of energy-related topics which are of special concern in the Department's long-range research efforts. Among the topics likely to be of concern in FY 1985 are combustion, bioconversion related to energy, nuclear waste isolation systems research, catalysis, advanced materials science and engineering, and the transport of energy-related pollutants. It is estimated that the $6,000,000 requested will enable the Department to assist about 10-20 institutions to obtain the specialized instrumentation required (items costing about $100,000 or more).

This program is complementary to and does not replace the Department's efforts to provide funds for scientific equipment required on individual research projects supported through the cognizant research programs. Requests for such instrumentation will continue to be included in research proposals submitted to the Department's basic and technology research programs.

The program will continue to be coordinated with similar programs in the other Federal agencies, including both proposals and awards. The close coordination ensures that each agency's program complements and reinforces the research efforts of all the agencies and makes each program more cost effective.

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DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
LEAD TABLE
ADVISORY AND OVERSIGHT PROGRAM DIRECTION
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
SUPPORTING RESEARCH AND TECHNICAL ANALYSIS
(Tabular dollars in thousands. Narrative material in whole dollars.)

	1983 Appropriation	1984 Appropriation	1985 Base	1985 Request
Energy Oversight, Research Analysis and University Support				
Advisory and Oversight Program Direction				
Operating Expenses	$ 2,603	$ 3,400	$ 3,400	$ 2,900
Total	2,603	3,400	3,400	2,900
Staffing Total FTE's:	45	44	44	44

Authorization: Section 209, P.L. 95-91.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
SUMMARY OF CHANGES
ADVISORY AND OVERSIGHT PROGRAM DIRECTION
(In thousands of dollars)

1984 Appropriation enacted	$ 3,400
Built in reduction	- 500
1985 budget request	$ 2,900

Advisory and Oversight Program Direction

The FY 1985 request for Advisory and Oversight Program Direction is $2,900,000, a decrease of $500,000 from the FY 1984 level. These funds are required to provide for the salaries, benefits, travel, and other expenses associated with 44 full-time equivalents. The funding reduction represents some management savings while at the same time continuing the FY 1984 staffing level.

This program provides the personnel resources required by the Director of Energy Research to carry out his responsibilities under legislation (P.L. 95-91) and as mandated by the Secretary in areas beyond the scope of the other assigned Energy Research programs. This staff performs in-house and external analyses and studies to meet the organization's responsibilities for monitoring the agency's research and development programs in order to advise the Secretary with respect to the well-being and management of the multiprogram laboratories. This responsibility includes advising on research activities carried out by any of the Assistant Secretaries; providing support for the Energy Research Advisory Board and Laboratory Management Council; and providing program management of the Energy Research Analysis, University Research Support, Multiprogram General Purpose Facilities (MGPF), and the University Research Instrumentation programs.

The FY 1985 request supports the following staff activities:

1. It will support the Director of Energy Research at the FY 1984 level of effort. The staff will continue to provide benefit studies of the results of research programs, evaluations of research that crosscuts programs for integration of objectives and approaches, and independent peer reviews of technical or research subjects as directed by the Secretary or other top management officials.

2. The university-laboratory research support and energy manpower development programs will continue to be supported. The principal goal is to help maintain strong scientific/technical research capabilities in support of the Department's long-range energy R&D mission in both the university community and the national laboratories. This is accomplished through specialized research and manpower development efforts which complement and support the R&D mission of other Departmental programs. The program provides a Departmental focus for several efforts which involve universities both directly or in conjunction with the national laboratories and major contractors.

3. The University Research Instrumentation program will continue to be supported. Staff effort includes such tasks as preparation of the program solicitation, analysis of proposals, selection of awards, and monitoring final implementation.

4. This staff will provide advice on the management and maintenance of the multiprogram nonweapons laboratories. The laboratory oversight role will include staff effort to implement the ERAB and OSTP recommendations for improved Departmental/laboratory relationships. The staff will serve as the Secretariat to an expanded, more effective Field Management Board which will review issues relating to the laboratories, and will manage the implementation of a more effective laboratory appraisal process by the operations offices. The staff will continue to prepare institutional plans for five ER multiprogram laboratories, carry out the institutional planning process for single purpose laboratories, manage the Multiprogram General Purpose Facilities program to revitalize the R&D facilities at the major laboratories, overview work performed by the national laboratories for outside agencies, conduct studies of the laboratory roles and relationships, and support the R&D Laboratory Technology Transfer Program.

5. The Energy Research Advisory Board will continue to be supported at the FY 1984 level.

6. Program and administrative support in the areas of budget and finance, personnel administration, policy and coordination, and construction management support will continue to be provided within this program.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
MAJOR ACTIVITY OVERVIEW

Multiprogram General Purpose Facilities

The goal of the Multiprogram General Purpose Facilities (MGPF) program is to provide for the rehabilitation and replacement of multiprogram general support facilities which are essential to the continued operations of the agency's multiprogram sites. Multiprogram General Purpose Facilities are facilities which are suited for and utilized by many different programs where no one program uses more than approximately 60 percent of the facility. These include roads, railroads, site utilities, and support buildings such as laboratories, office buildings, shops, warehouses, etc.

The following facilities and sites are included in the program:

Ames Laboratory
Argonne National Laboratory (ANL)
Brookhaven National Laboratory (BNL)
Hanford Engineering Development Laboratory (HEDL)
Idaho National Engineering Laboratory (INEL)
Lawrence Berkeley Laboratory (LBL)
Lawrence Livermore National Laboratory (LLNL)
Los Alamos National Laboratory (LANL)
Oak Ridge National Laboratory (ORNL)
Pacific Northwest Laboratory (PNL)
Richland Operations (RL)
Sandia National Laboratories (SNL)

These multiprogram sites received over $3,000,000,000 in FY 1983 to perform National research programs in nuclear energy, fusion energy, basic energy sciences, nuclear physics, high energy physics, life sciences, other energy-related areas, and defense systems. Over 50,000 contract personnel are engaged in these activities.

The replacement cost of the existing general purpose facilities at the multiprogram sites exceeds $6,500,000,000. The MGPF program is required to rehabilitate and/or replace deteriorated, non-functional facilities in a systematic and prioritized manner to ensure the continued effective accomplishment of DOE's R&D missions. The program helps alleviate the serious drain on R&D programs' operating budgets resulting from conducting work in old, worn out, out-moded and inefficient facilities.

The program is based on the premise that through continuous use and aging, facilities deteriorate over time to a point where they are no longer appropriate for their intended functions and must be rehabilitated or replaced. The program is an appropriate Federal role reflecting the responsible management of the Government's real property.

The program has accomplished the rehabilitation or replacement of numerous buildings, utilities, roads and railroads at the multiprogram laboratories since its establishment in FY 1981.

In FY 1984, the program, in addition to continuing projects previously approved, will initiate projects that:

- Rehabilitate utilities in the old town section of LBL.
- Replace cooling water towers at ORNL.
- Rehabilitate roads at LBL, INEL, RL and ANL.
- Replace a firehouse at BNL.
- Upgrade sewage treatment plant at ORNL.
- Rehabilitate water and waste treatment systems at ANL.

The specific objectives of the program from FY 1985 to FY 1989 are to rehabilitate and replace deficient facilities which are essential to the continued operations of multi-program sites, and to prolong the life of the Government's large investment in real property facilities at these sites.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
LEAD TABLE
MULTIPROGRAM GENERAL PURPOSE FACILITIES
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
(Tabular dollars in thousands. Narrative material in whole dollars.)

	1983 Appropriation	1984 Appropriation	1985 Base	1985 Request
Multiprogram General Purpose Facilities Construction	$ 34,000	$ 42,100	$ 42,100	$ 38,950
Total Construction	$ 34,000	$ 42,100	$ 42,100	$ 38,950

Authorization: Section 647, Public Law 95-91.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
SUMMARY OF CHANGES
ENERGY SUPPLY RESEARCH AND DEVELOPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(In thousands of dollars)

1984 Appropriation enacted	$ 42,100
1985 base	42,100
Program increases and decreases:	
o Add project for central chilled water facility at BNL	+ 3,500
o Add project to replace laboratory roofs at ANL	+ 3,508
o Add project to restore primary electrical distribution system at ORNL	+ 1,100
o Add project to rehabilitate underground steam system at ANL	+ 3,000
o Add project to replace and upgrade medical facilities at LLNL	+ 1,600
o Add project to replace site fire alarm system at RL	+ 1,300
o Add project to establish a central chilled water plant at ANL	+ 1,000
o Add project to upgrade environmental monitoring system at ORNL	+ 1,000
o Add project to replace independent chillers by increasing capacity at the central chilled water plant at ORNL	+ 1,000
o Planned additional funds required to complete project to rehabilitate LBL old town utilities	+ 2,750
o Planned additional funds required to complete the upgrade of the cooling water facility at ORNL	+ 2,800
o Planned additional funds required to complete the upgrade and improvements of roads at various laboratories	+ 1,500
o Planned decreases in project funding levels as projects are completed or near completion	-27,208
1985 budget request	$ 38,950

The FY 1985 request of $38,950,000 will allow continued rehabilitation, replacement and improvement of MGPF at the national laboratories, reflecting responsible management of the Government's real property and the importance of maintaining it adequately. The replacement costs of these prior investments is over $6 billion. This budget permits orderly reduction of over a billion dollar backlog of MGPF deficiencies; helps alleviate the serious drain on R&D programs' operating budgets resulting from conducting work in old, worn-out, out-moded and inefficient facilities; and provides for the continued effective accomplishment of DOE's R&D missions. The requested funding is summarized below by facility categories:

	FY 1984 BA (000)	FY 1985 BA (000)
Facility Categories:		
Buildings	$ 14,612	$ 9,358
Utilities	23,688	25,092
Roads	3,800	4,500
Total	$ 42,100	$ 38,950

The continued emphasis of the program is the upgrading of inadequate utility systems to acceptable levels of performance, reliability, and economy. Although overall the needs are greater in the buildings area (see discussion of backlog below), the projects with greatest urgency and potential impact for disrupting operations are in the utilities area.

A total of $21,942,000 is required to complete or continue funding of seven projects started in previous years. These projects are identified below:

On-Going		FY 1985 BA (000)
82-E-302	Security Facility, (ANL)	$ 1,100
83-E-308	Rehabilitate Power Systems, (INEL, LLNL, RL, ORNL)	2,842
83-E-309	Electronics Facility, (ANL)	3,150
83-E-310	Utility Replacement and Upgrade, (BNL)	3,200
84-ER-101	Rehab. Old Town Utilities, (LBL)	3,750
84-ER-102	Cooling Water Facility Rest., (ORNL)	3,400
84-ER-103	Road Repair (LBL, INEL, RL, ANL)	4,500
	Subtotal Ongoing	$ 21,942

The remainder of the request, $17,008,000 provides funds for the 9 new projects listed below:

New		TEC	FY 1985 BA (000)
85-R-701	Central Chilled Water Facility, (BNL)	15,000	3,500
85-R-702	Replace Laboratory Roofs, (ANL)	9,800	3,508
85-R-703	Electrical Distribution System Restoration (ORNL)	2,200	1,100
85-R-704	Rehab. Underground Steam System, (ANL)	3,000	3,000
85-R-706	Medical Facility Replacement (LLNL)	7,300	1,600
85-R-707	Replace Site Fire Alarm System (RL)	4,850	1,300
85-R-709	Establish a Central Chilled Water Plant (ANL)	5,200	1,000
85-R-711	Upgrade Environmental Monitoring (ORNL)	3,500	1,000
85-R-712	Modify Central Chilled Water Plant (ORNL)	4,700	1,000
	Subtotal New		17,008
	Total		$ 38,950

All new projects are consistent with the Department's Institutional and Site Plans for these laboratories and were selected as the highest priority projects from an extensive backlog of projects to correct the deficiencies at the laboratories. Construction Project Data Sheets which describe and justify each project in detail follow the narrative justification.

The MGPF program was established in FY 1981 to respond to the large backlog of facility support projects needed to maintain the adequacy of MGPF in fulfilling mission responsibilities. The backlog was quantified through a comprehensive inventory and assessment of all facilities at multiprogram sites in FY 1981. Each facility was surveyed and evaluated by experienced facility managers at the sites and deficiencies were identified, categorized and evaluated. Required minimum standards covering condition, capacity, location, safety and other factors were utilized to determine the extent of deficiencies. The consolidated results were reviewed and approved by field organization personnel and submitted to Headquarters. Annual updates of the list of projects needed to correct deficiencies are provided via the Preliminary Institutional Plans.

The inventory identified 17,000,000 square feet of laboratory/office space and 9,000,000 square feet of other support buildings such as shops, service centers, warehouses, garages, cafeterias, and other service buildings. Approximately 42 percent of the buildings are 30 years of age or older. Temporary facilities total almost 8 percent of the total inventory. Approximately 39 percent of the space is in poor or fair condition. Of the total work force 62 percent is housed in office areas of which half (16,000 persons) is considered to be in substandard office space or trailers. Similarly, many utility and road/railroad systems are old, out-moded, inefficient, uneconomical, and prone to failure.

Costs to Correct Deficiencies by Facility Category*
(in thousands of dollars)

Facility Use Category	Total Cost
Buildings	$ 805,000
Utilities	371,000
Roads, Railroads and Other Site Improvements	98,000
Total	$1,274,000

*Includes all needed projects regardless of size (i.e., those above and below $1,000,000).

Several factors contribute to the extensive backlog:

1. Inadequate Building Practices

Much of the agency's original physical plant was built during times of crisis when either shortages of materials or the urgency of the programs dictated utilizing inferior materials and/or rapid construction techniques. These practices have resulted in premature aging of some of the plant and expansion of routine maintenance to keep the plant on-line. More recently, as programs expanded, temporary facilities such as trailers and prefabricated buildings have been used in lieu of permanent facilities. These have a much shorter life span, and were contemplated to be temporary until more suitable facilities could be provided.

2. Aging and Deterioration

The aging and wear of facilities, particularly utility systems, affect the reliability of service and increase the downtime and routine maintenance costs for most systems. Real property at the laboratories averages 25 years with many of the facilities going back to the 1940's. Many of these buildings and utility systems have no remaining service life and must be replaced to continue operations at the laboratories.

3. Facility Support Lagged Operating Growth

Improvements to support facilities did not keep up with increases in R&D programs. The result is that existing facilities have been utilized well beyond their design capacities. This is especially noticeable in utility systems, roads, and laboratory facilities. Because adequate permanent facilities have not been available, the laboratories have, of necessity, converted space designed for other purposes (e.g., warehouse space) into laboratory space, and have continued to rely on World War II barrack type buildings which are limited in application and have leased offsite space in several instances. Such solutions can seldom provide the quality laboratory space needed to meet today's research standards.

4. Lack of Institutional Support for GPF

Prior to the MGPF program, the installations suffered from a lack of adequate institutional support largely because they accommodate many programs. All resident programs fund operating expenses to cover the work performed. However, only the assigned lead program (i.e., landlord) had been responsible in the past for providing general purpose facilities, which actually support many or all residing programs. More often than not, budget ceilings have prevented the lead program from accommodating both direct program requirements and institutional needs including general purpose facilities.

The impacts of these facilities' deficiencies are: increased operating costs; increased safety, security, health and environmental risks; greater likelihood of program interruption and delay; and low morale and productivity.

As part of the annual planning process for MGPF, several steps have been taken to assure that most of the above practices are not repeated.

1. The Institutional Planning and Site Development processes are designed to ensure orderly operation, maintenance, and growth (or reduction) of laboratories. These processes require consideration to be given to support facility needs prior to the introduction of any new program effort.

2. A more stringent and universally applied maintenance management system is being implemented to prevent the deferral of maintenance when it is detrimental to the physical well being of necessary facilities.

3. Better design criteria, earlier review of proposed facilities and more rigorous management during construction will be utilized for the MGPF program to keep the quality of construction high.

4. Finally, the planning and programming process utilized by the MGPF program will assure that the proper attention is paid to potential critical deficiencies so that they may be corrected prior to any serious impact on mission accomplishment.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 1st Qtr. FY 1986

4. Date Construction ends: 3rd Qtr. FY 1988

5. Previous cost Estimate: none
Date: none

6. Current cost estimate: $15,000
Less amount for PE&D: 0
Net cost estimate: $15,000
Date: September 1983

7. Financial Schedule:

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$15,000	$ 3,500	$ 3,500	$ 1,050
1986	0	7,500	7,500	4,850
1987	0	4,000	4,000	5,650
1988	0	0	0	3,450

8. Brief Physical Description of Project

This project proposes the construction of a central chilled water and compressed air facility. It will provide 5,100 tons of refrigeration and 1,500 standard cubic feet per minute (SCFM) of compressed air service for distribution to the following six major research complexes on site: Biology - Building 463; Medical Research Center - Building 490; Physics - Building 510; Applied Mathematics - Building 515; Laboratory Wings - Building 703; Hot Laboratory - Building 801.

The project consists of the installation of approximately 16,000 feet of underground chilled water piping and 8,000 feet of compressed air piping; the erection of one 5,100 ton capacity multicell cooling tower of complete fireproof construction and two buildings (a central chilled water and compressed air structure, and a condenser water pump house) having a total gross area of approximately 6,140 square feet and a gross volume of 115,100 cubic feet. Necessary switchgear at 13.8 KV, 2.4 KV and 480 volts, and a 500 KVA transformer substation are also included. Certain utility systems that interfere with construction will be extended, modified, or relocated; these include steam, water, electric power, telephone, and storm and sanitary drains. The present macadam service road (Temple Place) located adjacent to the central steam plant will be extended (20' x 50') in order to provide access to the proposed facility.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

8. Brief Physical Description of Project (continued)

The building identified as central chilled water and compressed air structure will be approximately 56' x 90' x 20' high. This building will abut and connect with the south wall elevation of the existing central steam facility.

The building will be approximately 5,040 square feet and will consist of slab-on-grade, steel framing, insulated sandwich wall siding with a built-up insulated roof deck.

The equipment level at grade will contain the following major refrigerations apparatus and associated components: Three 1,700 ton chillers, one 1,500 SCFM air compressor, three chilled water pumps, an automatic central control and monitoring system, electrical switchgear, motor control stations and associated piping and electrical lines.

The condenser water pump house of approximately 1,100 square feet will house two vertical condenser water pumps, and will be constructed with a slab-on-grade, concrete block walls, and built-up roof deck.

9. Purpose, Justification of Need for, and Scope of Project

This project is the most cost effective method for replacing major refrigeration and compressed air equipment that have become obsolete and beyond economical repair. The multiple independent systems that exist at Brookhaven National Laboratory historically have ever increasing operating and maintenance costs as the equipment ages. A new central chilled water facility would have lower maintenance and operating cost, and be able to maximize load diversity presently not possible with the independent building systems.

This project provides a firm base for substantial future reductions in capital construction, maintenance costs and energy consumption. In the future, work and spent individual air conditioning and compressed air systems in other scientific buildings will be replaced with chilled water and compressed air from the proposed central facility.

Background Profile of Existing Systems and Facilities

The existing decentralized systems of air conditioning, refrigeration, and compressed air are the result of each system being conceived as a self-contained entity as opposed to other basic utility services such as electrical power, potable water, waste water, steam, gas, etc., which are extended to a new facility from a central source. Chilled water, however, presently requires refrigeration units (centrifugal, steam absorption, etc.), cooling towers, pumps, electrical equipment, etc. to provide complete and independent systems for supplying environmental air conditioning to each building. This approach has resulted in a multiplicity of equipment and systems.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

9. Purpose, Justification of Need for, and Scope of Project (continued)

The major buildings are presently served by 36 units consisting of steam absorption, centrifugal and helical screw, refrigeration water chillers totaling 11,147 tons.

There are approximately 6,500 tons of additional refrigeration installed throughout various complexes. These range from small one-ton window air conditioning units to 150-ton reciprocating refrigeration assemblies.

Proposed Central Chilled Water Facility

It is proposed to construct a central chilled water and compressed air facility as a utility similar to other central facilities. The new chilled water plant will supply the refrigeration requirements for the six buildings and eliminate the use of well water used for once-through cooling at the Medical Research Center. The cooling systems being replaced were installed in the 1950s and 1960s and are obsolete, and beyond their normal life expectancy, and incur increasing operational and maintenance costs each year. In addition, this proposed facility would supply a source of clean, oil-free, low dewpoint compressed air for experimental and utility services within these facilities.

The proposed central chilled water and compressed air facility offers many tangible benefits over the multiplicity of the decentralized systems. Some of the major benefits are:

A. Permit new refrigeration systems to be installed at a lower initial cost ($360/ton) as compared with separate, independent systems ($790/ton).

B. Reduce operating and maintenance costs due to the elimination of independent chilled water and compressed air systems by centralization of major equipment.

C. Reduce capital installation costs due to utilization of load diversity among the various complexes.

D. Provide two additional proven wells for integration with the laboratory's potable and firefighting water supply system. The two existing wells in the Medical Research Center used for once-through cooling can be diverted to reinforce the domestic water system capacity.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

9. Purpose, Justification of Need for, and Scope of Project (Continued)

E. Provide for restructuring of the laboratory's present steam supply by removing from service the existing steam absorption machines (used for cooling). Approximately 148 million pounds of steam per year will be redeployed for better utilization (e.g., 20,000 lbs. of steam per hour for winter heating in lieu of winter air conditioning).

F. Permit the recycling of treated effluent from the central sewage facility for use as make-up at the central steam plant and the proposed central chilled water and compressed air plant. This would reduce the load on the potable water system by approximately 600 gpm.

G. Utilize the return tower condenser water to preheat boiler water make-up (approximately 25,000 GPD) at the Central Steam Facility conserving approximately 90 million pounds of steam a year (equal to saving 700,000 gallons of No. 6 fuel oil).

H. Reduce the energy costs at the six buildings by approximately 56% in today's dollars due to improved utilization and diversity source.

10. Details of Cost Estimate

	Item Cost		Total Cost
a. Architect-engineer, design and inspection at approximately 12% of construction costs, Item c			$ 1,400
b. Land and land rights			0
c. Construction costs			11,600
(1) Improvements to Land		$ 98	
Site preparation (L.S.)	$ 60		
Road and area surfacing, 1000 S.Y. @ $28	28		
Area lighting (L.S.)	10		
(2) Buildings (6,140 S.F. @ approximately $136)		833	

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

10. Details of Cost Estimate (continued)

	Item Cost	Total Cost
(3) Equipment (within buildings)		6,050
1700-ton machine (3) @ $516,000	$ 1,548	
Primary chilled water pumps (3) @ $39,000	117	
Secondary chilled water pumps (6) $14,000	84	
Air compressor (1)	187	
Chilled water, condenser, water, compressed air piping and miscellaneous accessories and equipment including six building tie-ins	2,789	
Condenser water pumps (2) @ $52,000	104	
Chemical water treatment system	91	
Automatic central control and monitoring system	905	
Electrical switchgear and distribution	225	
(4) Cooling Tower		536
(5) Utilities		4,083
Relocation of piping, electric lines, sewer and storm piping telephone, switchgear and distribution	932	
Chilled and condenser water supply and return piping	2,208	
Compressed air piping, valves (approximately 30 @ $6500), excavation, backfill, etc. for all underground utilities (10,000 ft. @ $46 per ft.)	943	
Subtotal		$13,000
d. Contingency @ approximately 15% of above costs		2,000
Total estimated cost		$15,000

11. Method of Performance

Design and inspection will be performed under a negotiated architect-engineer contract. Construction and procurement will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1985	FY 1986	FY 1987	FY 1988	Total
a. Total project costs						
1. Total facility costs						
(a) Construction line item ..	$ 0	$ 1,050	$ 4,850	$ 5,650	$ 3,450	$15,000
(b) PE&D	0	0	0	0	0	0
(d) Inventories	0	0	0	0	0	0
Total facility costs ..	0	$ 1,050	$ 4,850	$ 5,650	$ 3,450	$15,000
Total project costs	$ 0	$ 1,050	$ 4,850	$ 5,650	$ 3,450	$15,000

b. Other related annual costs (estimated life of project: 20 years)

1. Facility operating cost	$1,549,000
2. Programmatic operating expenses directly related to the facility	0
3. Capital equipment not related to construction but related to the programmatic effort of this facility	0
4. GPP or other construction related to the programmatic effort in the facility	0
5. Other costs	0
Total related annual costs	$1,549,000

The $1,549,000 annual operating cost is estimated as follows:

Maintenance and Operation	$ 317,000
Energy (Utilities)	1,232,000
Total operating costs	$1,549,000

However, if this facility is not funded, the existing systems in the six (6) buildings previously mentioned will have an annual operating cost as follows:

Maintenance and Operation	$ 578,000
Energy (Utilities)	2,341,000
Total operating costs	$2,919,000

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water facility
Brookhaven National Laboratory
Upton, New York

2. Project No.: 85-R-701

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

The annual savings of non-energy is $261,000 and energy is $1,109,000 for this proposed facility, when constructed.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding

1. Total Facility
   (a) Construction line item - Not required
   (b) CP&D - Not required
   (c) Expense funded equipment - Not required
   (d) Inventories - Not required

2. Other project funding
   (a) R&D necessary to complete - Not required
   (b) Other project related funding - Not required

3. Capital equipment not related to construction but related to the activity effort in the facility.
   Not required

4. GPP or other construction related to programmatic effort
   Not required

5. Other costs
   Not required

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Replace laboratory roofs
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-702

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 4th Qtr. FY 1985

4. Date construction ends: 4th Qtr. FY 1988

5. Previous cost estimate: none
Date: none

6. Current cost estimate: $ 9,800
Less amount for PE&D: 0
Net cost estimate: $ 9,800
Date: December 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 9,800	$ 3,508	$ 3,508	$ 2,030
1986	0	3,300	3,300	4,000
1987	0	2,992	2,992	3,770

8. Brief Physical Description of Project

The proposed project will replace built-up membrane roofs on principal general purpose laboratory buildings, giving priority to existing conditions. Approximately 880,000 sq. ft. of roof will be replaced. The work will consist of stripping existing membrane and insulaton where conditions require, patching decks as required, improving drainage by compensating for low spots, installing new current technology membranes designed to best fit field conditions, adding insulation to bring heat transfer resistance up to current DOE standards, and, finally, providing protection to the membranes from temperature extremes and actinic attack. Flashings, curbs, gravel stops, and facias will be renewed as their conditions dictate. Satisfactory function of roofing components will be warranted for 10 years, directly by the material manufacturers.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Replace laboratory roofs
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-702

9. Purpose, Justification of Need for, and Scope of Project

The purposes of this project are to restore the weather tightness of roofs on laboratory buildings, and to bring the resistance to heat transfer up to current Federal energy use standards. This project provides a multi-year plan, described in the ANL Institutional Plan, FY 1983-FY 1985, whose goal is the replacement of all roofs older than 25 years on permanent general purpose buildings. At this age they have exceeded normal life expectancy for conventional built-up membrane construction. Resources expended on reconditioning efforts exceed good business judgment, yet the research programs housed under the roofs have been impacted.

Total replacement is required. Programs housed in these buildings include Basic Energy Research, Fossil Energy Research, Conservation, Renewable Energy, Environmental Protection, Safety, and Emergency Preparedness. Twenty one buildings are scheduled with approximately 880,000 square feet of roof needing immediate attention.

10. Details of Cost Estimate

ANL has replaced over 70,000 square feet of roofs since 1982 under five separate competitively bid contracts. In addition to the roof area, the amount of roof and insulation to be removed, the relative number of roof penetrations and other complications to be provided all produced a range of unit prices from $6.03 to $8.68 per square foot when normalized to mid-1982. The mean unit cost derived from these bids was $7.30 in mid-1982.

The various elements contributing to the total unit cost of roof replacement are identified in the following table:

Job Cost Breakdown

Cost Element	$ Per Sq Ft Mid-1982
Tear-off of old roof and insulation (90% of roof area)	$1.34
Preparation of substrate	0.38
Improve water drainage (average)	1.04
Single-ply PVC membrane	1.48
Irma Board - 2" thick insulation	2.04
Pro-rated edge and penetration details (average)	1.02
Warranties (included in above costs)	--
Estimated total	$7.30

1. Title and location of project: Replace laboratory roofs
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-702

10. Details of Cost Estimate (continued)

The following estimated total cost of the project is for the construction of approximately 200,000 square feet for four years, 80,000 square feet in the last year of the project. The above unit cost of $7.30 in mid-1982 has been escalated for each annual increment of construction, using the escalation rates projected below.*

	Total Cost
a. Engineering, design and inspection at approximately 11% of construction, Item b.	$ 900
b. Construction costs, 880,000 sq. ft. @ $10.80/sq. ft.	8,000
c. Contingency @ approximately 10% of above costs	900
Total estimated project cost	$ 9,800

*Based upon a completed conceptual design and current cost data.

11. Method of Performance

Engineering, design and inspection will be performed by laboratory engineering personnel. Construction will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1985	FY 1986	FY 1987	Total
a. Total project costs					
1. Total facility costs					
(a) Construction line item ..	0	$ 2,030	$ 4,000	$ 3,770	$ 9,800
(b) PE&D	0	0	0	0	0
(c) Expense funded equipment.	0	0	0	0	0
(d) Inventories	0	0	0	0	0
Total facility costs .	0	$ 2,030	$ 4,000	$ 3,770	$ 9,800

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Replace laboratory roofs
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-702

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

2. Other project costs					
(a) R&D necessary to complete construction	0	0	0	0	0
(b) Other project related costs	8	0	0	0	8
Total other project costs	$ 8	$ 0	$ 0	$ 0	$ 8
Total project costs (Items 1 and 2)	$ 8	$ 2,030	$ 4,000	$ 3,770	$ 9,808

b. Other related annual costs (estimated life of project: 20 years)

1. Facility operating costs	0
2. Programmatic operating expenses directly related to the facility	0
3. Capital equipment not related to construction but related to the programmatic effort in the facility	0
4. GPP or other construction related to programmatic effort in the facility	0
5. Other costs	0
Total other related annual costs	0

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
1. Total Facility
(a) Construction line item - No narrative required
(b) PE&D - None
(c) Expense funded equipment - None
(d) Inventories - None

2. Other project funding
(a) No R&D effort is required
(b) $8,000 spent for Conceptual Design

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Replace laboratory roofs
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-702

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

b. Total related funding requirements

The roofing components to be replaced or rehabilitated will have useful lifetimes of approximately 20 years.

1. Facility operating costs

Implementation of this project will rehabilitate or replace physical components of buildings. This will result in a reduction of maintenance costs while restoring the respective system components to an acceptable level of operational efficiency, thus the facility operating cost is reported as zero.

2. Programmatic operating expenses directly related to the facility

Although this project will rehabilitate general purpose facilities employed to perform a wide variety of activities, there is no programmatic operating expense directly related to, or required for supply of this project, thus the programmatic operating expenses is reported at zero.

3. Capital equipment not related to construction but related to the programmatic effort in the facility - None

4. Maintenance, repair, GPP or other construction related to programmatic effort - None

5. Other costs - None

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Primary electrical distribution system restoration
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-703

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 4th Qtr. FY 1985

4. Date Construction ends: 4th Qtr. FY 1987

5. Previous cost Estimate:
Date: none

6. Current cost estimate: $ 2,200
Less amount for PE&D: 0
Net cost estimate: $ 2,200

Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 2,200	$ 1,100	$ 1,100	$ 660
1986	0	1,100	1,100	1,000
1987	0	0	0	540

8. Brief Physical Description of Project

This project will involve a series of restoration activities which will increase the reliability of the existing electrical distribution system to an appropriate level. These activities will include repair or replacement of deteriorated components, replacement of deficient items, and the elimination of potential safety and environmental hazards. Deteriorated equipment to be replaced includes wooden poles, transformers, and cables. Correction of deficiencies include replacing fused disconnect switches with electrically-operated circuit breakers, improving lightning protection of overhead lines, and replacement of single-pole switches with three-pole switches. Correction of potential safety hazards includes additional isolation switches for buildings and facilities and improved relaying. Correction of potential environmental hazards includes replacing deteriorated liquid-filled (oil and PCB) transformers.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Primary electrical distribution system restoration
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-703

9. Purpose, Justification of Need for, and Scope of Project

This project will renew and upgrade the existing primary electrical distribution system to an appropriate level of reliability and enable it to effectively support various research activities at the Laboratory. Much of this system at Oak Ridge National Laboratory (ORNL) was built in 1943. Many of the components are beyond their expected life and are showing clear evidence of deterioration to the point where an escalating number of failures are projected. Examples of this deterioration are: (1) several oil filled transformers which have become severely corroded internally due to moisture and acid content will be replaced; (2) fused disconnect switches will be replaced with the electrically operated circuit breakers; (3) unshielded cable which is in violation to the National Electric Code will be replaced with approved shielded cable; (4) lightning protection will be improved on those circuits supplying the High Flux Isotope Reactor, Transuranium Processing Plant, Health Physics Research Reactor and to the Tower Shielding Facility thereby increasing the reliability of these circuits.

In addition, single pole switches will be replaced with three pole switches. This change will allow operating personnel to be better utilized during emergency conditions and reduce switching time which results from waiting for called in maintenance personnel.

The cost estimate is based on a conceptual design completed during FY 1982 and will be issued during FY 1983 at an estimated cost of $20,000.

10. Details of Cost Estimate*

	Item Cost	Total Cost
a. Engineering, design, and inspection at approximately 13% of construction costs, item b		$ 220
b. Construction costs		1,720
(1) Outside utilities	$, 1,720	
Subtotal		$ 1,940
c. Contingency at approximately 15% of above costs		260
Total Project Cost		$ 2,200

*Based on a Conceptual Design Report completed in FY 1982 at a cost of approximately $20,000.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Primary electrical distribution system restoration
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-703

11. Method of Performance

Design and inspection will be performed under a negotiated architect-engineer contract. Construction and procurement will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

Not Required. TEC is less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not Required. TEC is less than $5,000,000.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Rehabilitate underground steam system
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-704

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 4th Qtr. FY 1985

4. Date Construction ends: 4th Qtr. FY 1987

5. Previous cost Estimate: none
Date: none

6. Current cost estimate: $ 3,000
Less amount for PE&D: 0
Net cost estimate: $ 3,000
Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 3,000	$ 3,000	$ 3,000	$ 1,000
1986	0	0	0	1,000
1987	0	0	0	1,000

8. Brief Physical Description of Project

The project provides for rehabilitation of approximately 3350 lineal feet of steam distribution system. Together with work completed since 1978, this plan will complete reconditioning of the entire underground tunnel. The work includes:

a. Replacing deteriorated reinforced concrete tunnel covers with extended precast covers to provide walkthrough maintenance, securing against ground water infiltration with waterproof membrane.

b. Providing under-drains along the sides of the tunnel to aid in ground water removal; alternately, where existing under-drain is usable, rehabilitate to assure free water flow.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate underground steam system
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-704

8. Brief Physical Description of Project (continued)

c. Replacing all pipe anchors, pipe guides and pipe rollers including associated concrete bases.

d. Replacing corroded or leading steam supply and condensate return piping.

e. Providing additional 2 inches of heavy density thermal insulation on the 12 inch high pressure steam supply piping and rewrapping with protective material.

f. Applying 2 inches of heavy density thermal insulation to the condensate return piping and wrapping with protective material.

g. Reconditioning existing manholes by replacing defective concrete, waterproofing exteriors, and replacing defective pipe insulation.

The project schedule and the associated financial schedule reflects an assessment of reasonable funding expectation plus an evaluation of the impact of construction on laboratory activities.

9. Purpose, Justification of Need for, and Scope of Project

a. The present underground distribution system is over 30 years old, contains many worn out parts and is subject to unpredictable and frequent breakdowns. Common conditions are deteriorating and crumbling concrete, rusted parts, corroded and eroded pipes, anchors, guide bases, roller bases and valves, and leaking tunnel covers. Condensate return lines are presently not insulated and there is significant energy loss from these lines. Ground water leaking into the tunnel is accelerating deterioration of both concrete and steel components. Poor access design requires digging up and disassembling the tunnel covers to perform any inspection, maintenance, or repair work of the piping system.

b. Rehabilitation of the steam distribution system will assure continued reliability of the steam supply.

Expected benefits are:

(1) Improved reliability in maintaining steam supply to ten major scientific facilities.

(2) Reduction in maintenance and repair costs for steam distribution.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate underground steam system
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-704

9. Purpose, Justification of Need for, and Scope of Project (continued)

c. A portion of the project has finite cost return potential:

Reduction of steam energy losses by retrofitting and applying new insulation. The system has been analyzed by a recognized computer service. The calculated pay back period for the insulation portion of the work is less than 5 years for both lines. The heat loss on the steam line will be reduced from 200 BTU/hr/lineal ft to 117 on the steam line, or a 41% reduction. The heat loss on the condensate line will be reduced from 122 BTU/hr/lineal ft. to 14 or an 89% reduction.

The plan for rehabilitation of the underground steam system is consistent with the five year plan for plant rehabilitation described in the ANL Institutional Plan, FY 1983-1988.

10. Details of Cost Estimate:*

	Total Cost
a. Engineering, design and inspection at approximately 17% of construction, Item b	$ 340
b. Construction costs	2,120
c. Contingency @ approximately 21% of above costs	540
Total Estimated Project Cost	$ 3,000

11. Method of Performance

Engineering, design and inspection will be performed by laboratory engineering personnel. Construction will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

Not Required. TEC less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not Required. TEC less than $5,000,000.

*Based upon a completed conceptual design and current cost data.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Hanford site fire alarm system upgrade
Richland, Washington

2. Project No.: 85-R-707

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 2nd Qtr. FY 1986

4. Date construction ends: 2nd Qtr. FY 1987

5. Previous cost estimate: none
Date: none

6. Current cost estimate: $ 4,850
Less amount for PE&D: 0
Net cost estimate: $ 4,850
Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 4,850	$ 1,300	$ 1,300	$ 840
1986	0	3,550	3,550	2,145
1987	0	0	0	1,865

8. Brief Physical Description of Project

This project provides for the design, procurement and construction of an upgraded fire alarm system which will be commensurate with required levels of protection for the Hanford Site. The project will replace all existing master alarm boxes and street boxes with radio boxes, replace alarm receiving equipment and consoles at the fire stations, and provide a computer aided dispatch system.

This project will replace approximately 240 master alarm boxes and 50 street boxes, which are distributed throughout the site. This will require additional equipment to interface the new master boxes with the existing detector circuits in the facilities. The existing alarm receiving equipment at the fire stations will be replaced with new equipment compatible with the new alarm boxes. Significant features of the new alarm receiving equipment includes English printout of facility location and alarming zone within the facility. This equipment will be supplemented with a new computer aided dispatching system. This will increase the efficiency of responding emergency personnel by providing information not available with the existing system. This includes information such as type of occupancy, recommended extinguishing agents, and adjacent conditions.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Hanford site fire alarm system upgrade
Richland, Washington

2. Project No.: 85-R-707

9. Purpose, Justification of Need for, and Scope of Project

The purpose of this project is to update the existing fire alarm system with a more reliable and efficient system. There has been no significant overhaul of the Hanford fire alarm system since the site was originally established in the early 1940's. Some system components are approaching 50 years in age. Repair of components is difficult at best due to the lack of spare parts. Overhead conductors are generally in excess of 20 years old with significant amounts in excess of 30 years old. Due to the normal aging process the insulation of these conductors is brittle and breaks easily leaving conductors exposed and permitting faults in the system. In some locations, alarms are transmitted to the fire stations on underground conductors. Major portions of these lines are uncharted and are subject to dig-ups during construction and maintenance activities.

Due to deterioration and age of the system components, numerous false and nuisance alarms as well as ground faults occur. Records of alarm signals for calendar years 1979, 1980 and 1981 indicate alarms due to electrical problems, malfunctions, atmospheric phenomenon, and equipment failures ranged between 28 and 37 percent of the total number of alarms received. It is estimated that the proposed system could eliminate 50 percent of these alarms.

As the facilities at the site have been increased in size as well as number, additions to the fire alarm reporting system have been made to cover them. Unfortunately, by necessity, requirements of the National Fire Codes have been violated. These violations concern connection of detectors to master alarm boxes in an unacceptable manner, inadequate annunciation, and inappropriate alarm receiving at the fire stations.

The need for the fire alarm system upgrade is based on an audit report done in June 1982 by Diliberto and Associates, consultants specializing in fire protection and safety engineering. The audit report identifies 30 categories of deficiencies within the existing fire alarm system. An Engineering Study, also by Diliberto and Associates, addressed alternative solutions for correcting existing deficiencies. Through the site survey by Diliberto and Associates, overall system analysis, and the consultant's fire alarm system expertise, it was concluded that to achieve compliance with NFPA, ensure system reliability, future flexibility and ease of operation, a Radio fire alarm system alone fulfilled these requirements.

Delay of this project will increase the risk of serious fire accidents due to continued aging of the system and its components. Also, maintenance costs of the existing system will continue to increase.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Hanford site fire alarm system upgrade, Richland, Washington

2. Project No.: 85-R-707

10. Details of Cost Estimate*

	Item Cost	Total Cost
a. Engineering design and inspection at approximately 13% of construction costs		$ 500
b. Construction costs		3,720
(1) Construction (includes equipment and labor)	$ 1,910	
c. Standard equipment includes 6 consoles ($54,000/ea.) computer aided dispatch system ($204,000) and approximately 278 radio alarm boxes ($4,600/ea.)	1,810	
Subtotal		$ 4,220
d. Contingency at approximately 15% of above cost		630
Total Project Cost		$ 4,850

11. Method of Performance

Design, inspection, and construction will be accomplished by fixed-price contracts awarded on the basis of competitive bidding. It will be a design, procure and install contract as presently planned.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

Not required. TEC is less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not required. TEC is less than $5,000,000.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES

(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Central chilled water plant
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-709

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 2nd Qtr. FY 1986

4. Date Construction ends: 4th Qtr. FY 1987

5. Previous cost Estimate: none
Date: none

6. Current cost estimate: $ 5,200
Less amount for PE&D: 0
Net cost estimate: $ 5,200
Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 5,200	$ 1,000	$ 1,000	$ 750
1986	0	4,200	4,200	3,000
1987	0	0	0	1,450

8. Brief Physical Description of Project

This project establishes a central water chilling plant to serve all the principal buildings in the central research group. Two new electric centrifugal chillers totaling 3200 tons are planned for a now-unoccupied area of the former ZGS facilities. Use is made of existing cooling towers, pumps, piping, and electrical power. Approximately 3 miles of chilled water supply and return piping are routed to the user buildings. Local terminal connections are included. The connecting pipeline is specified as uninsulated, corrosion-resistant plastic pipe, buried below frost line. New chilled water circulation pumps are included for the control facility, with necessary pump modifications of the terminal delivery points.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water plant
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-709

9. Purpose, Justification of Need for, and Scope of Project

The proposed project offers an integrated, cost-saving alternate to piecemeal replacing of worn out water chillers. The water chillers installed during construction of the Laboratory are beyond their normal life expectancy; to maintain active research operations, the ANL Institutional Plan, 1983-1988, identifies a nearly $6,000,000 program of chiller replacement. By establishing a central water chilling plant, greater reliability and more economical operations are possible. A 1977 ANL engineering study aimed at integrated water chilling facilities identified the savings and also pointed to savings possible by retiring steam-driven chillers in favor of electrical. However, when combined with the unavoidable necessity of replacing worn out chillers, the central plant concept is definitely attractive, offering both immediate benefits and greatly enhanced potentials. The annual estimated savings in energy, repair, and maintenance, in 1983 dollars, is approximately $500,000 for providing a central chilled water plant to replace eight existing steam driven chillers in the above mentioned four buildings.

In addition to the benefits of central chilled water supply, this project makes use of existing facilities: i.e., the vacant area in Building 370 and the under-utilized electric substations and pumped cooling tower water lines from the cooling tower near Building 370. If these under-utilized facilities were not available, a new building for the central chillers complete with new cooling towers, pumps, and electrical substation would have to be constructed at an additional cost to the project of $763,000. The capacity built into the existing facilities will accommodate the central chilling concept, yet allow a generous margin to attract future research programs. Superimposing the water chilling function offers assurance that the existing facilities will remain profitably available in good condition.

10. Details of Cost Estimate

	Item Cost	Total Cost
a. Engineering, design and inspection at 15.6% of construction, Item b.		$ 600
b. Construction costs		3,270
(1) Valve pits	$ 135	
(2) Trenching and backfill	460	
(3) Buried chilled water piping	1,280	
(4) Piping and equipment within buildings	1,170	
(5) Controls and metering	60	
(6) Electrical power for chillers and pumps	165	

*Based upon a completed conceptual design and current cost data.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water plant
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-709

10. Details of Cost Estimate (Continued)

c. Procurement costs (chillers, primary pumps & strainer)	600
d. Contingency - 16.6% of engineering, construction & procurement	730
Total Estimated Project Cost	$ 5,200

11. Method of Performance

Engineering, design and inspection will be performed by laboratory engineering personnel, aided by outside A/E firms. Construction will be accomplished by fixed-price contract awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1985	FY 1986	FY 1987	Total
a. Total project costs					
1. Total facility costs					
(a) Construction line item	$ 0	$ 750	$ 3,000	$ 1,450	$ 5,200
(b) PE&D	0	0	0	0	0
(c) Expense funded equipment	0	0	0	0	0
(d) Inventories	0	0	0	0	0
Total facility costs	$ 0	$ 750	$ 3,000	$ 1,450	$ 5,200
2. Other project costs					
(a) R&D necessary to complete construction	0	0	0	0	0
(b) Other project related costs	20	0	0	0	20
Total other project costs	$ 0	$ 0	$ 0	$ 0	$ 0
(Items 1 and 2)	$ 20	$ 750	$ 3,000	$ 1,450	$ 5,220

1642

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Central chilled water plant
Argonne National Laboratory
Argonne, Illinois

2. Project No.: 85-R-709

12. Funding Schedule of Project Funding and Other Related Funding Requirements (Continued)

b. Total related funding requirements (estimated life of project: 20 years) - N/A

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
1. Total facility costs (N/A)

2. Other project funding
(a) No R&D effort is required
(b) $20,000 spent for Conceptual Design

b. Total related funding requirements

The central water chilling facility to be established will have a useful lifetime upwards of 20 years.

1. Facility operating costs

Implementation of this project will replace existing physical functions within individual buildings with a central plant. This will result in a reduction of maintenance and operating costs while restoring an acceptable level of operational efficiency to existing facilities, thus the facility operating cost is reported as zero.

2. Activity operating expenses directly related to the facility

Although this project will restore and replace general purpose facilities employed to perform a wide variety of activities, there is no activity operating expense directly related to, or required for support of this project, thus the activity operating expense is reported as zero.

3. Capital equipment not related to construction but related to the activity effort in the facility - None.

4. GPP or other construction related to activity effort - None

5. Other costs - None

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Upgrade environmental monitoring systems
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-711

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 1st Qtr. FY 1986

4. Date Construction ends: 4th Qtr. FY 1988

5. Previous cost Estimate: none
Date: none

6. Current cost estimate: $ 3,500
Less amount for PE&D: 0
Net cost estimate: $ 3,500
Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 3,500	$ 1,000	$ 1,000	$ 300
1986	0	2,500	2,500	1,150
1987	0	0	0	1,300
1988	0	0	0	750

8. Brief Physical Description of Project

The purpose of the proposed project is to modernize existing liquid and gaseous environmental monitoring stations at Oak Ridge National Laboratory (ORNL); to add additional stations to provide more detailed coverage of the surrounding area; and to provide new data handling capabilities. The monitoring information will be transmitted to a central location for processing and analysis. As presently envisioned, the work will include the following:

A. Gaseous Effluents

(1) Reinstrument selected existing air monitoring stations and add new stations. Stations will be instrumented for radioiodine, wet and dry radioactive fallout, and radioparticulate collection. Stations may also be equipped with thermoluminescent dosimeters, and will perform air concentration determinations for alpha- and beta-gamma particulates and noble gas activity. Continuous radioisotopic analysis, tritium gas monitoring and SO_2 monitoring may be performed at selected stations.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Upgrade environmental monitoring systems
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-711

8. Brief Physical Description of Projects (Continued)

(2) Add real-time, representative stack-gas monitoring-complex system(s) at one or more existing off-gas stacks to provide isotopic analyses of radionuclides. Near real-time data will be telemetered as required.

B. Liquid Effluents

(1) Reinstrument selected existing and add new proportional sampling stations. Proportional sampling stations will include one near the Melton Hill Dam and one downstream of the ORNL complex.

(2) Add continuous liquid effluent monitoring systems. These systems may be located at White Oak Creek.

C. Data Collection and Analysis

Install a computerized system to receive parametric and diagnostic information from the liquid and gaseous monitoring stations. Central readout panels will be provided.

9. Purpose, Justification of Need for, and Scope of Project

A. General

It is the Department of Energy (DOE) policy, stated in DOE Orders 5480.1 and 5484.1, that all off-site effluents be reduced to "as low as reasonable achievable" levels. The ORNL monitoring systems that were installed 25 years ago are insufficient in precision and are unable to measure the specific effluents that are required by the DOE Orders. The 25 year old monitoring instrumentation presently in use has inherent background levels which are too high to permit required measurements at current levels. Further improvements in keeping with the "as low as reasonably achievable" requirement will require more sensitive instrumentation. Such instrumentation is commercially available at this time. The proposed computerized system will be used to analyze and compare the data with past norms to provide early indications of long-term trends that may be developing.

The present instrumentation is also inadequate to predict with either reasonable accuracy or adequate time the consequences of an unplanned release from the Laboratory. Only a few gross parameters are measured at ORNL's discharge points and in the environment. Very little of this information is telemetered for processing and analysis, so that it could be used in responding to such a release.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Upgrade environmental monitoring systems
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-711

9. Purpose, Justification of Need for, and Scope of Project

B. Air Monitoring System Replacement

The root cause of the deficiencies in the air monitoring systems is the age of the stations themselves. They use vacuum-tube electronics which are 25 years old and reliable parts are no longer available. Some replacement parts require frequent replacement (e.g., as often as once a month for certain vacuum tubes). Other deficiencies include overall station deterioration and the need to increase the number of monitored variables and the number of monitoring stations to fill gaps in the current arrays. The solution to these problems is to replace the vacuum-tube electronics with commercially available, modular, solid state units.

Finally, additional instrumentation (e.g., real-time stack monitoring) are required to have both an accurate knowledge of source terms and environmental concentrations for routine and accidental releases and to provide a basis for controlling emissions to an "as low as reasonable achievable" level.

C. Water Monitoring System Replacement

The existing on-site and off-site monitors and proportional samples need to be reinstrumented because of the obsolete electronics presently used in these systems. Proportional sampling stations are needed to get an accurate sample proportional to flow at a point upstream and downstream of ORNL discharges and where the water is first used for public consumption. These replacements will enable ORNL to comply with DOE Orders 5480.1 and 5484.1.

D. Data Processing and Analysis

Data from radiation and non-radiological monitors will be telemetered for processing, analysis and archiving on a routine or emergency basis. The data processing and analysis system may also serve as a back-up system for ORNL's Waste Operation Control Center and as a predictive tool in the event of an unplanned release.

Additional instrumentation is needed to monitor for non-radiological pollutants.

Modernization of existing liquid and gaseous environmental monitoring stations could be conducted in phases over several years with alternative capital funds; however, implementation of multiple designs, procurement packages and construction contracts as well as integrating separately designed and installed systems would lead to inefficiencies and higher costs. In addition, due to the shortage of General Purpose Plant (GPP) and General Purpose Equipment (GPE) funds, this approach would be difficult to accomplish.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Upgrade environmental monitoring systems
Oak Ridge National Laboratory
Oak Ridge, Tennessee

2. Project No.: 85-R-711

9. Purpose, Justification of Need for, and Scope of Project (Continued)

Another alternative is to continue to operate with the present 25 year old systems which, as discussed above, would present increasing operational and maintenance problems; moreover, the inadequacies of the current systems would not be resolved.

10. Details of Cost Estimates*

	Item Cost	Total Cost
a. Engineering, design, and inspection at approximately 12% of construction costs, item b.		$ 350
b. Construction costs		2,800
(1) Data acquisition (including facility adaptation)	$ 1,300	
(2) Special facilities (gaseous effluents)	1,100	
(3) Special facilities (liquids effluents)	400	
Subtotal		$ 3,150
c. Contingency at approximately 12% of above costs		350
Total Project Cost		$ 3,500

* Estimate based on a completed Conceptual Design Report.

11. Method of Performance

Design and inspection will be by negotiated architect-engineer contract. To the extent feasible, construction and procurement will be accomplished by fixed-price subcontracts and prime contracts awarded on the basis of competitive bidding. The data acquisition system will be specified and procured according to DOE regulations and requirements.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

Not Required. TEC is less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not Required. TEC is less than $5,000,000.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Central chilled water system restoration
Oak Ridge National Laboratory, Tennessee

2. Project No.: 85-R-712

3. Date A-E work initiated: 1st Qtr. FY 1985

3a. Date physical construction starts: 1st Qtr. FY 1986

4. Date construction ends: 4th Qtr. FY 1988

5. Previous cost estimate: None
Date: None

6. Current cost estimate: $ 4,700
Less amount for CP&D: 0
Net cost estimate: $ 4,700

Date: September 1983

7. Financial Schedule

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1985	$ 4,700	$ 1,000	$ 1,000	$ 510
1986	0	3,700	3,700	1,570
1987	0	0	0	1,730
1988	0	0	0	890

8. Brief Physical Description of Project

This project will remove from service three obsolete 600 ton chiller units located in the Central Research and Administration Complex and provide replacement capacity. The Central Compressor Facility structure will be expanded, if required, for the installation of 2,000 ton centrifugal chiller and the associated pumps, controls, and piping. Concurrently, the cooling tower system supplying condenser water to the facility will be upgraded to correct a marginal capacity condition during peak demand periods.

9. Purpose, Justification of Need for, and Scope of Project

The purpose of this project is to: replace three 600 ton chiller units due to age, condition, and limited capacity; increase capacity of a marginal cooling tower system.

The Central Research and Administration Complex consists of seven major facilities with approximately 1,000,000 sq. ft. of floor space and approximately a third of the Laboratories' research personnel. The space is used by multi-discipline groups and supporting service divisions participating in applied and basic research programs.

1. Title and location of project: Central chilled water system restoration
Oak Ridge National Laboratory, Tennessee

2. Project No.: 85-R-712

9. Purpose, Justification of Need for, and Scope of Project (continued)

The units to be replaced were obtained from surplus channels in 1952 and are now approximately 35 years old. Their reliability continues to decline, and, in recent years, two of the three machines have been out of service for several weeks or more. Repair parts are no longer stocked by the manufacturer and downtimes are extended by the need to custom fabricate the necessary parts.

The declining reliability of these machines will continue and more frequent interruptions and greater delays to programmatic activities can be anticipated. Many programmatic activities are dependent on computer services and the ORNL Computer Center located in the area served by the 600 ton chillers.

10. Details of Cost Estimate*

	Item Cost	Total Cost
a. Engineering, design, and inspection at approximately 12% of construction costs, item b.		$ 450
b. Construction costs		3,700
(1) Land improvements including grading, landscaping	$ 43	
(2) Building addition (2,500 sq. ft. @ $153/sq. ft.)	362	
(3) Building modifications (concrete work, etc.)	131	
(4) Other structures (cooling tower)	419	
(5) Special facilities (chiller, pumps, piping, etc.)	2,745	
Subtotal		$ 4,150
c. Contingency at approximately 15% of above costs		550
Total Project Cost		$ 4,700

*Cost estimate based on completed conceptual design.

11. Method of Performance

Design and inspection will be on the basis of a negotiated architect-engineer contract. Construction and procurement will be accomplished by fixed-price contracts and subcontracts awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

Not required. TEC is less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not required. TEC is less than $5,000,000.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Rehabilitate old town area utilities
Lawrence Berkeley Laboratory,
Berkeley, California

2. Project No.: 84-ER-101

3. Date A-E work initiated: 2nd Qtr. FY 1984

3a. Date physical construction starts: 3rd Qtr. FY 1985

4. Date construction ends: 2nd Qtr. FY 1986

5. Previous cost estimate: None
Date:

6. Current cost estimate: $ 4,750
Date: March 1982

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1984	$ 4,750	$ 1,000	$ 1,000	$ 400
1985	0	3,750	3,750	2,400
1986	0	0	0	1,950

8. Brief Physical Description of Project

This project consists of the rehabilitation, replacement or improvement of the aged plant utilities systems serving a multiprogram array of research and development facilities in the oldest portion of the Lawrence Berkeley Laboratory. This old original area of the Laboratory which was generally constructed in the 1940's and early 50's encompasses 26 buildings with a total area of about 145,000 GSF as well as the major utilities load centers and primary distribution mains which serve this old area and peripheral shops and support facilities. Piecemeal development over several decades coupled with the super-imposition of heavy user R&D programs has resulted in overloaded, outdated and deteriorated utilities systems with inadequate reliability and flexibility.

This project will include comprehensive analysis and design to upgrade or replace selected load centers, distribution mains and components to rehabilitate the following utilities systems.

- Water service; domestic, industrial and low conductivity systems including new cooling towers, lift pumps, circulating pumps and demineralizers, instruments and controls. About 3000 lineal feet of pipe (various sizes) will be replaced or relocated along with valves, hydrants and control stations.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate old town area utilities
Lawrence Berkeley Laboratory,
Berkeley, California

2. Project No.: 84-ER-101

8. Brief Physical Description of Project (continued)

- o Compressed air service; about 4800 lineal feet (various sizes) will be replaced or relocated along with valves, control stations and a standby air compressor control system.
- o Natural gas service; about 2600 lineal feet will be replaced or relocated. New pressure reducing stations, meters, earthquake shut-off valves and vaults will be included.
- o Electrical service; about 800 lineal feet of primary and secondary low voltage and high voltage distribution will be replaced or relocated along with two sub-stations with transformers and switch gear, manholes, conduit, new motor control centers and energy monitoring and control systems components. One new centrally located standby generator will replace five old unreliable army surplus generators and provide peak shaving capacity to reduce demand costs.
- o Communications service; including new duct banks, conduits and manholes for telephones, public address, fire alarm and energy monitoring and control systems.
- o Sanitary sewerage; about 3820 lineal feet (various sizes) will be replaced or relocated.
- o Storm sewerage; about 2800 lineal feet (various sizes) will be replaced or relocated.

Generally, rehabilitation will provide improved flexibility, capacity, reliability and backup and reduce energy use and maintenance costs. An important feature of the project will involve consolidating main runs of various utilities into a new utilities and service road corridor through the "Old Town" area. This corridor will provide optimum accessibility for utilities maintenance, modification and program flexibility as well as a badly needed thoroughfare to improve traffic circulation and reduce safety hazards.

The conceptual design for this project is consistent with the proposed redevelopment plan for the "Old Town" area which is the keystone of LBL's long range development plan.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate old town area utilities
Lawrence Berkeley Laboratory,
Berkeley, California

2. Project No.: 84-ER-101

9. Purpose, Justification of Need for, and Scope of Project

The old original area of the Laboratory which was developed during a 10 year period which began about 40 years ago includes 26 buildings with heavy and light laboratories, shops, and high bay facilities which are intensely used for multiprogram research and development. A number of these programs also provide vital single source technology and development support for national research programs at other DOE installations. This area of the LBL site is also the prime functional and physical location for future utilization of the Laboratory's scientific resources. Due primarily to age, the existing utilities systems in "Old Town" are in an advanced state of deterioration; corroded, overloaded and unreliable with inadequate flexibility to handle varying programmatic demands. Many components of the electrical systems date back well before the Lawrence Laboratory began. Many were originally acquired from army surplus. Currently, utilities breakdowns, systems leaks and service problems plague research schedules and place heavy demands on LBL's Plant Maintenance resources. Frequently, natural gas leaks, power problems, corroded waste lines and antiquated components of these systems cause serious safety problems for operations personnel and pose environmental hazards. Rehabilitation is urgently required to avoid serious disruption to R&D schedules and to mitigate safety and environmental hazards.

The Magnetic Fusion Energy (MFE) and Biomedical Programs must depend on the "Old Town" Utilities systems for their continued accomplishment. These programs are funded at approximately $15M per year and require the direct utilization of approximately 150 scientific and support personnel. An added dimension to the support picture for "Old Town" area of LBL utilities is that major Magnetic Fusion Energy (MFE) projects at Lawrence Livermore National Laboratory (LLNL), Princeton Plasma Physics Laboratory and General Atomics are dependent upon work on neutral beams conducted in the "Old Town" area. These projects are the Mirror Fusion Test Facility at LLNL, the Tokamak Fusion Test Reactor at PPPL, and the Doublet III at General Atomic.

Annual operating costs upon completion of this project are expected to total $60,000, about $15,000 for maintenance and $45,000 for energy. This represents a decrease of $100,000 in annual maintenance costs and $20,000 in annual energy costs.

This project will be constructed at the Lawrence Berkeley Laboratory which is non-Government owned property.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate old town area utilities
Lawrence Berkeley Laboratory,
Berkeley, California

2. Project No.: 84-ER-101

10. Details of Cost Estimate*

	Item Cost	Total Cost
a. Engineering, design and inspection at about 15% of construction cost		$ 560
b. Construction costs:		3,760
1. Site work (Civil)	$ 570	
2. Site utilities	1,540	
3. Mechanical utilities	410	
4. Electrical utilities	1,240	
Subtotal		4,320
c. Contingencies at about 10% (of which $376,000 is for construction)		430
Total estimated cost		$ 4,750

* Estimate is based on completed Conceptual Design.

11. Methods of Performance

Engineering design will be performed under a negotiated Architect/Engineer subcontract. Inspection and some engineering will be done by LBL personnel. Construction and procurement will be accomplished by fixed price subcontracts awarded on the basis of competitive bids.

12. Funding Schedule

Not required because the total estimated cost of this project is less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not required because the total estimated cost of this project is less than $5,000,000.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Cooling water facilities restoration
Oak Ridge National Laboratory, Tennessee

2. Project No.: 84-ER-102

3. Date A-E work initiated: 1st Qtr. FY 1984

3a. Date physical construction starts: 1st Qtr. FY 1985

4. Date construction ends: 4th Qtr. FY 1986

5. Previous cost estimate: None
Date:

6. Current cost estimate: $ 4,000
Date: April 1982

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1984	$ 4,000	$ 600	$ 600	$ 300
1985	0	3,400	3,400	2,000
1986	0	0	0	1,700

8. Brief Physical Description of Project

The project will provide for restoration of a 38-year-old cooling system presently serving Oak Ridge National Laboratory (ORNL) research buildings in the Y-12 Plant area. These buildings contain Fusion Energy Division research and development experiments, Engineering Technology Division facilities in support of fission reactor development and safety programs, and the ORNL Isotope Separation Operations. The existing cooling tower with extended coil shed will be demolished and removed from the existing cooling tower basin. A new multi-cell cooling tower will be added on the existing tower basin and any excess basin area will be covered with span decking. The work will include separate high and low pressure demineralized heat exchangers. Some of the piping serving the tower will be refurbished or replaced. Structural modifications will be required to the existing foundations to make them compatible with the new tower. Underground electrical power and control service to the tower and pumphouse will be provided as well as fire protection.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Cooling water facilities restoration
Oak Ridge National Laboratory, Tennessee

2. Project No.: 84-ER-102

9. Purpose, Justification of Need for, and Scope of Project

The purpose of this project is to provide for restoration and refurnishment of the existing, inadequate and unreliable cooling water system presently serving ORNL Multi-Program Research within building 9201-2 at the Y-12 Plant.

ORNL facilities located in Building 9201-2 in the Y-12 Plant were constructed in the early 1940's to house electromagnetic separation equipment. Since 1959, these facilities have undergone extensive and numerous internal renovations and modifications to make them functional for their changing application in support of multiple programs of ORNL. Currently, three major divisions of the Laboratory have exclusive use of these facilities for key programs which are central to the mission of ORNL as a major contributor to energy-related research. In terms of floor space, no one program dominates and all presently contemplated uses of these facilities continue to be multi-programmatic.

The cooling water utilities system currently serving the ORNL research facilities in Building 9201-2 is operating at only 30% of the systems initial capability. With this limitation the system's present cooling capacity is 15MW thermal. The current operating load is 22 MW thermal. To compensate for this shortfall of 7MW the Fusion Energy, Energy Technology, and Isotope Separation Programs are restricted to operation on a selective scheduling basis. The requirement for selective scheduling coupled with increased system down time for maintenance is seriously restricting operation of these facilities. The significance of the maintenance effort for this system is evidenced by the cost. In 1981 maintenance costs exceeded $200,000 and are projected to reach $300,000 for 1982. In addition to these costs the structural deterioration of the cooling tower has created hazardous working conditions for maintenance personnel.

10. Details of Cost Estimate*

	Item Cost	Total Cost
a. Engineering, design, and inspection at approximately 12% of construction costs, item b. ...		$ 375
b. Construction costs		3,150
(1) Other structures	$ 3,150	
Subtotal		3,525
c. Contingency at approximately 13% of above costs		475
Total Project Cost		$ 4,000

* Costs are extracted from the Conceptual Engineering Design prepared by Burns & Roe Industrial Services, Inc., and as adjusted by UCC-ND Engineering.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Cooling water facilities restoration
Oak Ridge National Laboratory, Tennessee

2. Project No.: 84-ER-102

11. Method of Performance

Design and inspection will be based on a negotiated architect-engineer contract. Construction and procurement will be accomplished by fixed-price prime contract awarded on the basis of competitive bidding.

12. Funding Schedule for Project Funding and Other Related Funding Requirements

Not required because the total estimated cost of this project is less than $5,000,000.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

Not required because the total estimated cost of this project is less than $5,000,000.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Road repair, various locations (ANL, INEL, LBL, RL)

2. Project No.: 84-ER-103

3. Date A-E work initiated: 2nd Qtr. FY 1984

3a. Date physical construction starts: 4th Qtr. FY 1984

4. Date construction ends: 1st Qtr. FY 1987

5. Previous cost estimate: None
Date: June 1982

6. Current cost estimate: $16,000
Less amount of PE&D: 0
Net Cost Estimate: $16,000
Date: August 1982

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1984	$ 16,000	$ 3,000	$ 3,000	$ 1,000
1985	0	4,500	4,500	3,600
1986	0	8,500	8,500	4,600
1987	0	0	0	4,800
1988	0	0	0	2,000

8. Brief Physical Description of Project

This project is for the restoration, widening, and improvement of roads at various sites to improve traffic safety and bring these roads into conformance with current standards and practices in highway construction. Brief descriptions of each component, by site, follows:

A. Traffic Safety Improvements, Route 4, Richland, Washington - Approximately six miles of Route 4, the arterial road servicing the Hanford area, will be improved to be more consistent with Washington State highway design guidelines. Each lane will be widened approximately 2 feet to provide standard 12-foot lanes. Shoulder surfaces will be treated and widened to provide the standard design width. Acceleration, deceleration, and holding lanes will be provided where required.

Safety hazards such as poles, fire hydrants, and telephone cable boxes will be removed or relocated as required. Appropriate traffic control devices, lane markers, guard rails, roadway signs, pavement markings, and crash protection will be provided as necessary. The road shall be resurfaced with an asphalt overlay to eliminate the cracked and uneven places and to match and blend with the additions proposed by this project. The intended useful life of this project is 25 years.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Road repair, various locations (ANL, INEL, LBL, RL)

2. Project No.: 84-ER-103

8. Brief Physical Description of Project (continued)

B. INEL Road Refurbishment, Idaho National Engineering Laboratory (INEL), Idaho - This project provides for restoring approximately 37 miles of INEL primary and secondary roads to a safe and reliable condition. The project design will provide an engineered road cross section meeting traffic density and load requirements. Since this is not a total reconstruction project, the repair methods will vary from applying an asphaltic leveling course on the existing surface to demolishing and reconstructing the total road cross section. The work method selected will depend on conditions along the route of each section to be restored. The completed roads will have painted traffic striping, proper crown, adequate surface-thickness, engineered base-course, compacted subgrade and side drainage.

C. Roadwork Project - Safety Program, Lawrence Berkeley Laboratory (LBL), Berkeley, California - This project provides for increasing the radius of curves at various intersections and widening of the main access road to the Laboratory. Vertical and horizontal curves will be removed and roads realigned to conform to the Department of Transportation Highway Design Standard. Included will be separation of pedestrian and vehicular traffic in some areas of the complex.

D. Repair Existing Roads, Argonne National Laboratory (ANL), Argonne, Illinois - This project will reconstruct approximately 10 miles of roadway serving the ANL-East Laboratory site. Included in this reconstruction effort are the main entrance routes to the site and those roads serving the principal permanent buildings and facilities. Roads serving buildings that are to be deactivated will not be reconstructed.

Work to be performed includes:

a. Repair of base course failures
b. Resurfacing with 2-1/2 inch bituminous concrete topping
c. Rework and repair of road shoulders
d. Raising existing manholes to match new road alterations
e. Restriping of traffic lanes and crosswalks
f. Replacement of deteriorated culvert pipes

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Road repair, various locations (ANL, INEL, LBL, RL)

2. Project No.: 84-ER-103

9. Purpose, Justification of Need for, and Scope of Project:

A. Traffic Safety Improvements, Route 4, Richland, Washington - Route 4 is the arterial servicing the Hanford Site. This roadway was built in 1943 prior to formalization of national policies on highway design. Lack of conformance to current highway design guidelines has created serious traffic hazards on the Hanford Site. In addition, Route 4 has deteriorated over the years. The road surface is cracked and uneven, lanes are narrow, and in most places the shoulders are soft, narrow and rutted. The existing lanes are only 10 feet wide, 2 feet narrower than required by current standards. The 10-foot lanes allow very little maneuvering room, and create heavy traffic loads along the road edge. This stress causes pavement edge break-up and hence further reduction of lane width, and deep ruts in the shoulders. These factors have caused increased maintenance and safety problems. This project proposes to improve that portion of Route 4 from the 1100 Area to the gravel pit, a distance of approximately 6 miles. This area carries the greatest amount of traffic and has the highest accident rate.

B. INEL Road Refurbishment, Idaho National Engineering Laboratory (INEL), Idaho - The roads proposed for reconstruction are the sole access to active INEL facility areas. They have been maintained in continuous use since their original construction during the 1950's and 1960's. Maintenance efforts since that time have included patching, seal coating and surface overlays. Deterioration in the base course and subgrade has progressed to the point that these efforts provide only short term improvement. In addition, pavement edge-breakage has narrowed the road in some sections to less than the minimum required for safe two-lane operation. The current situation has resulted from combinations of the following circumstances:

- Existing roads that were not designed for current traffic density and loads which have led to continuing surface and subsurface breakdown.
- Extreme winter cold temperatures ranging to -40°F causing surface course brittleness and shrinkage leading to extensive cracking, subsequent moisture penetration and subsurface failure.
- High summer temperatures ranging to 100°F causing road weakness in areas of minimum road stability. This results in ruts, depressions and washboards on the road surface.
- Moisture entry through surface cracks and unpaved shoulders. This causes reduced subsurface support strength and surface breaking.
- Frost heave caused by soil capillarity and poor drainage during winter weather. This results in both surface breakup and subsurface failure.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Road repair, various locations (ANL, INEL, LBL, RL)

2. Project No.: 84-ER-103

9. Purpose, Justification of Need for, and Scope of Project (continued)

C. Road Project - Safety Program, Lawrence Berkeley (LBL), Berkeley, California - The existing radius of the curves of the main access road to the laboratory are such that semi-trailers are found to go over the road center line. In some areas of the laboratory pedestrians and vehicles must use the same road way.

Improvement of the laboratory roading and pedestrian systems are required to bring the old substandard roads and sidewalks in the hilly LBL terrain up to acceptable code and safety standards by improving alignment sight distance, removing horizontal and vertical curves, increasing the radius of curves and widening the access road to the site.

This project will be constructed at the Lawrence Berkeley Laboratory which is non-Government owned property.

D. Repair Existing Roads, Phase I, Argonne National Laboratory (ANL), Argonne, Illinois - The site roads are deteriorating at a faster rate than they can be economically repaired. This deterioration reflects the age of the roads, approximately 30 years, and the severity of the climate at the ANL-East site. Failing road edges, the result of base course failures and late winter thaws, cannot be corrected by patching methods. The use of operating funds in an attempt to maintain the roadways in serviceable condition has resulted in unsatisfactory road conditions at best, and a heavy drain on the Laboratory's resources.

A full reconstruction program for those sections of the roadway network which are in worst condition will be provided by this project.

10. Details of Cost Estimate*

	Richland	INEL	LBL	ANL	Total
a. Engineering and design and inspection	$ 530	$ 535	$ 165	$ 200	$ 1,430
b. Construction costs	3,840	6,110	1,045	1,600	12,595
Subtotal	4,370	6,645	1,210	1,800	14,025
c. Contingency	630	955	190	200	1,975
Total Project Cost	$ 5,000	$ 7,600	$ 1,400	$ 2,000	$16,000

*Conceptual Design Reports completed.

1. Title and location of project: Road repair, various locations (ANL, INEL, LBL, RL) 2. Project No.: 84-ER-103

11. Method of Performance

A. RL Subproject - Design and inspection will be accomplished by a negotiated architect-engineering contract or the on-site architect-engineer firm. The major portion of the construction will be accomplished under fixed-price contracts awarded on the basis of competitive bids. Relocation of any power or utility poles will be accomplished through negotiations with the appropriate utility.

B. INEL Subproject - Overall responsibilities for design and construction will be assigned to the INEL prime contractors administered by DOE-ID. The INEL contractor will provide technical direction of the design effort. Construction will be accomplished by fixed price subcontracts awarded on the basis of competitive bidding.

C. LBL Subproject - Design and inspection will be performed under a negotiated architect-engineer contract. To the extent feasible, construction and procurement will be accomplished by fixed-price contracts and subcontract awarded on the basis of competitive bidding.

D. ANL Subproject - Engineering, design and inspection will be performed by Laboratory engineering personnel. Construction will be accomplished by fixed-price contract awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	Total
a. Total project costs							
1. Total facility costs							
(a) Construction line item	$ 0	$ 1,000	$ 3,600	$ 4,600	$ 4,800	$ 2,000	$16,000
(b) PE&D	0	0	0	0	0	0	0
(c) Expense funded equipment	0	0	0	0	0	0	0
(d) Inventories	0	0	0	0	0	0	0
Total facility costs	$ 0	$ 1,000	$ 3,600	$ 4,600	$ 4,800	$ 2,000	$16,000
2. Other project funding							
(a) R&D necessary to complete construction	$ 30	$ 0	$ 0	$ 0	$ 0	$ 0	$ 30
(b) Other project related costs	0	0	0	0	0	0	0
Total other project funding	30	0	0	0	0	0	0
Total project funding (1 and 2)	$ 30	$ 1,000	$ 3,600	$ 4,600	$ 4,800	$ 2,000	$16,030

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL)

2. Project No.: 83-E-308

3. Date A-E work initiated: 1st Qtr. FY 1983

3a. Date physical construction starts: 2nd Qtr. FY 1984

4. Date construction ends: 4th Qtr. FY 1985

5. Previous cost estimate: None

6. Current cost estimate: $15,830
Less amount of PE&D: 0
Net Cost Estimate: $15,830
Date: April 1981

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1983	$ 5,000	$ 5,000	$ 5,000	$ 1,000
1984	10,830	7,988	7,988	3,800
1985	0	2,842	2,842	9,400
1986	0	0	0	1,630

8. Brief Physical Description of Project

This project rehabilitates parts of the electrical power distribution systems at the four agency locations listed below:

- o Idaho National Engineering Laboratory (INEL)
- o Lawrence Livermore National Laboratory (LLNL)
- o 300 Area of Richland Site (RL)
- o Oak Ridge National Laboratory

The subprojects are described below:

Power Systems Rehabilitation, INEL - This project provides for correcting existing deficiencies in the main substation and in three of the area substations. Improvements to the main substation include replacing three main-feed 138,000-Volt oil circuit breakers which will not have sufficient fault current interrupting capacity by 1983. Lightning arrestors will be installed to provide proper surge protection for the Central Facility area-substation transformers colocated with the main substation. An additional oil circuit breaker will be installed to provide for isolating a long distribution line from the circuit supplying nearby area buildings. Additional switches, grounding, foundations, and hardware will be included to provide the needed improvements.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

8. Brief Physical Description of the Project (continued)

Three area substations remote from the main substation will receive system protection improvements including lightning arrestors, grounding, fencing, and hardware to adequately protect existing transformers from voltage surges. Also included will be the conversion of ungrounded (delta) distribution lines to an effectively grounded system with special transformers, resistors, and earth connections. A relaying system will be added to detect ground faults and to automatically isolate the faulted portion of the system utilizing existing circuit breakers.

Main Substation Transformer, LLNL - This subproject will consist of a new 115 kV - 13.8 kV, 3 phase transformer rated at 100 MVA, FOA (Forced Oil Assist). Associated equipment will include the necessary primary switchgear, lightning arrestors and buss supported on a low profile steel structure. Secondary switchgear will be housed in an addition located between Buildings 424 and 425.

13.8 Kilovolt Distribution Upgrade, RL - This project will upgrade existing substation C3-S4 in the southern part of the 300 Area to a 13.8 kilovolt (kV) switching station. The switching station will consist of fourteen metalclad switchgear cubicles in a prefabricated metal building with an underground cable vault. Ten 13.8 kV circuit breakers will be installed leaving space for two additional breakers as replacement facilities are added in this vicinity. The remaining two cubicles will house control and metering equipment. Approximately 900 meters of underground duct banks and associated access manholes will also be installed to provide orderly circuit exits from the substation and integrated routing to existing, new and planned replacement facilities. Abandoned poles will be removed and their 13.8 kV and 2.4 kV cables will be relocated to the underground duct banks.

Rehabilitate Electrical Service, ORNL - This subproject will provide for upgrading the 30-year-old electrical power system presently serving Oak Ridge National Laboratory (ORNL) research buildings in the Y-12 Plant area. It will provide for a new substation with a 50 MVA transformer to serve all the research experiments using the large DC motor-generator sets. The new transformer will be connected to a 161 kV unregulated feeder. The present 50 MVA transformer will be retained to provide emergency backup through secondary switchgear and will normally serve only the smaller, steady building loads from a 161 kV regulated feeder. A new oil circuit breaker will be installed in the main 161 kV Y-12 substation to provide switching of the regulated and unregulated 161 kV feeders for the two transformers.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

9. Purpose, Justification of Need for, and Scope of Project

Power System Upgrade, INEL - The INEL is supplied with electric power from the Northwest Power Transmission System through three high-voltage lines owned by major utility companies. The three lines converge at a utility-owned transformer substation within the INEL. This substation reduces the supply to 138,000 Volts which is fed to the nearby Government-owned main INEL substation. This latter substation connects with the east and west terminations of the 63-mile long Government-owned INEL power loop. The substation and five remote area-substations provide the sole source of commercially generated electric power for the 893-square-mile INEL.

The existing main substation oil circuit breakers (OCB's) were installed during the original construction of the site in the 1950's. The installed short-circuit interrupting capacity was adequate for the many years that the power-grid fault-capacity was less than 1,500 megaVoltAmperes. Presently, if a short-circuit were to occur, the OCB's may not interrupt the fault and could fail. This failure could result in a total loss of power to the INEL if destruction was accompanied by the failure of additional equipment. In any case, the reactor facilities would not have a redundant power source and could not operate until the systems could be repaired, which is estimated to be four months.

The original substation design did not provide adequate protection for high-voltage surges. In many cases, lightning arrestors were not installed. The overhead ground conductors on the 138,000-Volt lines provide shielding from direct strikes. Surges are still experienced, however, from normal switching and when induced by nearby lightning strikes. In addition, the low voltage lines do not have shielding. Continuing to expose the transformers to high voltage surges can only result in decreased transformer life and ultimate failure. At best, this would destroy power supply redundancy for reliable operation. At worse, multiple failures could leave one or more INEL areas without electricity for an extended time.

Much of the INEL area distribution system was designed using the three-wire (delta) ungrounded concept. This was a conventional system that was intended to be able to maintain power continuity despite a single conductor-to-ground fault. Widespread experience in the United States has shown that both reliability and safety are significantly lower in actual practice. Utility companies are quickly converting similar distribution systems to grounded systems to solve continuing problems.

The lack of an effective ground on three-wire systems sets up the condition for potentially destructive high-voltage transients. This was experienced between August 21 and 29, 1979, when electrical incidents occurred, which resulted in a total power outage at one INEL major reactor facility. This total power outage resulted in major work stoppage with personnel being sent home. As a result of these incidents, an investigating committee was appointed to determine the cause of the incidents and to make recommendations for avoiding similar occurrences. The committee

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

9. Purpose, Justification of Need for, and Scope of Project (continued)

concluded that the cause of equipment failure was excessive over voltage caused by an arcing ground fault. The proper system grounding and protective relaying would have cleared the faulted circuit rather than causing the total system loss. On January 8, 1980, another power outage occurred at the same reactor facility. The incident resulted in melted bus bars and cracked bus bar supports. This incident is considered to have further aggravated the latent damage done during the previous incidents. Outages such as occurred in August and January at the affected facility may occur during or while preparation for a nuclear experiment is going on. The programmatic impact and accompanying financial losses implied are in the millions of dollars. Further review of all INEL areas disclosed that similar risks exist. This project will correct existing problems.

Main Substation Transformer, LLNL - Electric power for LLNL and the Sandia Livermore Laboratory is provided by means of a 115 kV overhead transmission line from Pacific Gas and Electric's Tesla substation. Incoming 115 kV power is stepped up to a site distribution voltage of 13.8 kV by the three transformers in the main substation.

Current site electrical loads are carried by transformer No. 700 (56.0 MVA) and transformer No. 400 (22.5 MVA). In 1978, transformer No. 700 failed and was under repairs for approximately one month. During this month, transformer No. 400 was utilized in conjunction with transformer No. 100 (40 MVA) to carry the site load. Transformer No. 100 is now dedicated to Magnetic Fusion Energy (MFE) pulsing loads. A failure of transformer No. 700 today would require a shutdown of the MFE experimental work or a shedding of approximately 50% of the site load or some combination of both. The seriousness of the situation is compounded by the fact that the estimated order-to-delivery time for a replacement transformer is about 10 months.

Installation of the proposed new main substation transformer will eliminate the potential for a major electrical outage at LLNL and the Sandia Livermore Laboratory and will accommodate possible future increases in electrical demand.

13.8 Kilovolt Distribution Upgrade, Richland - This project upgrades the existing electrical distribution system in the 300 Area to increase the reliability and maintenance flexibility, and provide access to the system for replacement facilities being constructed in the southern portion of the area.

The 13.8 kV bus extension via expansion of the existing substation C3-S4 (Building 352-F) accomplishes the following:

- Provides switching capability allowing access to electrical systems through a substation rather than direct line tapping as is now necessary.

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

9. Purpose, Justification of Need for, and Scope of Project (continued)

- o Increases operating flexibility for load transfers during maintenance activities without interruption of customer service.

Undergrounding the overhead line accomplished the following:

- o Increases the reliability by establishing feeder positions for loads on the "power corridors."
- o Provides switching and terminal connections for designated planned loads for replacement facilities in the south end of the 300 Area.
- o Separates normal and emergency power and communications circuits on a common pole line, serving the same facility. Major facilities affected include:
  - 331 Complex, where loss of power would destroy laboratory animals requiring delicate temperature control and other empirical data from ongoing biological experiments, at high cost.
  - 320 Building, a classified atmospheric physics laboratory with critical ventilation (white room) requirements and sensitive computers which cannot tolerate power variance.
- o Eliminates the risk of a total power, fire alarm, and telephone outage, from a single pole failure.
- o Eliminates overhead line interference with beneficial use of prime real estate for proposed new facilities. Two major facilities have already been forced to relocate their site plans resulting in the existing pole line crossing parking lots.
- o Allows orderly site development preventing the electrical distribution system in the South end of the 300 Area from becoming as congested, inaccessible and unmaintainable as the electrical system in the North end.
- o Complies with the 300 Area Site Planning to underground all utilities in southern part of 300 Area.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

9. Purpose, Justification of Need for, and Scope of Project (continued)

ORNL facilities located in the Y-12 Plant were constructed in the early 1940's to house electromagnetic separation equipment. Since 1959, these buildings have undergone extensive and numerous internal renovations and modifications to make them functional for their changing application in support of multiple programs of ORNL. Currently, three major divisions of the Laboratory have exclusive use of these facilities for key programs which are central to the mission of ORNL as a major contributor to energy-related research.

Electrical power service to the research facilities is currently provided via one 50 MVA transformer approximately 27 years old. Testing of this transformer by maintenance has revealed deterioration of the transformer. The tests as conducted by maintenance and known as Doble Tests which are nationally known and accepted tests for determining the deterioration in transformers over their expected life cycle. The consequences of this transformer failing are serious because it takes 12 - 24 months to repair or replace the units and the 20 MVA back-up transformer is not sufficient for 12 - 24 months operation until a new transformer would be available. In the back-up mode several Fusion Energy and Engineering Technology Programs would be seriously curtailed and two programs could not operate. In addition the operations of the Isotope Separation Program would be severely restricted. The programs which would be impacted by failure of the existing transformer are currently funded at over $30,000,000/Year (Staff of over 180). There currently are no surplus or spare power transformers of this capacity in the Oak Ridge Operations area. Major ongoing ORNL research programs would be stopped or seriously curtailed until repairs could be made.

Of further significance is the fact brought out in the engineering assessment that all three large power transformer failures which have occurred in Y-12 were in substations supplying ORNL facilities were large motor-generator (MG) sets were operating. Eight large MG sets of similar design are in operation and are connected to the 50 MVA transformer. It is apparent that these large MG sets operating in Y-12 have contributed to the frequency and severity of power transformers and switchgear faults. Past maintenance data shows that the reliability of transformer supplying the ORNL facilities in Y-12 where large MG sets are operating is not as high as the reliability of transformers serving the remainder of Y-12, ORGDP, and the TVA system. Given this degree of lower reliability in combination with the seriousness of consequences if the 50 MVA transformer fails, the risks of failure are higher than justifiable. The proposed upgrade will provide reliable, cost-effective electrical utilities to adequately support agency operations at the ORNL research facilities in the Y-12 plant.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

10. Details of Cost Estimate*

	INEL	LLNL	Richland	ORNL	Total
a. Engineering and Design and Inspection	460	225	200	600	1,485
b. Construction Costs	3,780	1,525	3,200	3,700	12,205
Subtotal	4,240	1,750	3,400	4,300	13,690
c. Contingency (overall approximately 15.6%)	660	180	600	700	2,140
Total	4,900	1,930	4,000	5,000	15,830

*The cost estimates are based on completed conceptual designs.

11. Method of Performance

LLNL Subproject
Design will be on the basis of a negotiated architect-engineer contract. Major equipment requiring lead time will be purchased by LLNL early in the project on the basis of competitive bidding. To the extent feasible, construction will be accomplished by a fixed-price contract awarded on the basis of competitive bidding. Minor architect-engineering work and activiation will be performed by UC-LLNL forces.

INEL Subproject
The responsibility for design and project management will be assigned to the INEL Prime Contractor under administration by agency-ID. Construction will be accomplished by contracts and subcontracts awarded on the basis of competitive bidding.

RL Subproject
Design and inspection will be by negotiated architect-engineer contract. Construction will be accomplished by fixed-price subcontracts which are awarded on the basis of competitive bids. The fixed-price contractor will procure the major engineered equipment.

ORNL Subproject
Design and inspection will be based on a negotiated architect-engineer contract. Construction and procurement will be accomplished by fixed-price prime contract awarded on the basis of competitive bidding.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1983	FY 1984	FY 1985	FY 1986	Total
a. Total project costs:						
1. Total facility costs:						
(a) Construction line item	$ 0	$ 1,000	$ 3,800	$ 9,400	$ 1,630	$15,830
(b) PE&D	0	0	0	0	0	0
(c) Expense funded equipment	0	0	0	0	0	0
(d) Inventories	0	0	0	0	0	0
Total facility costs	$ 0	$ 1,000	$ 3,800	$ 9,400	$ 1,630	$15,830
2. Other project costs						
(a) R&D necessary to complete construction	$ 0	$ 0	$ 0	$ 0	$ 0	$ 0
(b) Conceptual design costs*	110	0	0	0	0	110
Total other project costs	110	0	0	0	0	110
Total project costs (Items 1 and 2)	$ 110	$ 1,000	$ 3,800	$ 9,400	$ 1,630	$15,940

b. Other related annual costs (estimated life: 30 years)	
1. Facility operating costs	$ 175
2. Programmatic operating expenses directly related to the facility	0
3. Capital equipment not related to construction but related to the programmatic effort	0
4. GPP or other construction related to the programmatic effort in the facility	0
5. Other costs	0
Total other related annual costs	$ 175

*Conceptual Design Reports completed.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Rehabilitate power systems, various locations (INEL, LLNL, ORNL, RL) 2. Project No.: 83-E-308

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
   1. Total facility costs
      (a) Construction line item - no narrative required
      (b) PE&D - no narrative required
      (c) Expense funded equipment - no narrative required
      (d) Inventories - no narrative required
   2. Other project funding
      (a) R&D necessary to complete construction - no narrative required
      (b) Conceptual design costs - Conceptual designs were completed in the fourth quarter of FY 1981 at a cost of $110,000.

b. Total related funding requirements
   The useful life of these facilities for programmatic purposes is 30 years.
   1. Facility operating costs - $175,000.
   2. Programmatic operating expenses directly related to the facility - The programmatic operating expenses are based on personnel costs. None
   3. Capital equipment not related to construction but related to the programmatic effort - None
   4. GPP or other construction related to the programmatic effort in the facility - no narrative required.
   5. Other costs - no narrative required.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Electronics facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 83-E-309

3. Date A-E work initiated: 1st Qtr. FY 1983

3a. Date physical construction starts: 1st Qtr. FY 1984

4. Date construction ends: 4th Qtr. FY 1985

5. Previous cost estimate: None

6. Current cost estimate: $ 8,500
Less amount of PE&D: 0
Net Cost Estimate: $ 8,500
Date: January 1981

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1983	$ 1,200	$ 1,200	$ 1,200	$ 240
1984	7,300	4,150	4,150	1,600
1985	0	3,150	3,150	5,150
1986	0	0	0	1,510

8. Brief Physical Description of Project

This project provides approximately 57,000 gross square feet of space for the Electronics Division (EL) at ANL/East and people from other divisions whose work interacts on a continual day-to-day basis with Electronics Division, a total of 111 personnel. Of the 57,000 square feet total, approximately 12,000 square feet are for mechanical equipment, penthouses and other utility areas. To promote technical interaction, the new building will be sited in close proximity to the Applied Mathematics Division.

The new building will have two above-grade floors and a full service floor. The design will assure economical delivery, handling and storage of electronic components, apparatus and supplies. Exterior architectural design will be aesthetically compatible with existing 200-area buildings. Construction will be masonry curtain wall with structural steel frame; special electrical considerations will be included; and the building envelope, fenestration and mechanical systems will be designed for maximum life cycle costed energy efficiency.

Corridor, stairwell and toilet room walls will be concrete block. Partitioning systems compatible with use, flexibility, and life cycle cost will be installed in other areas. Acoustical ceilings will be used throughout, except in storeroom and mechanical equipment areas on the service floor and in the toilet rooms and locker rooms.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Electronics facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 83-E-309

8. Brief Physical Description of Project (continued)

Parking areas to accommodate approximately 70 vehicles and access roads to the building entrance and loading dock will be provided. Concrete walks will be installed as required.

The cost of demolishing vacated structures and removing the debris is included in the total project cost.

9. Purpose, Justification of Need For, and Scope of Project

The purpose of this project is to provide for the replacement of the existing buildings, 817 and 818, now housing the Electronics Division. The severe age-deteriorated condition of the existing facilities severely hampers operations and the ability to service Laboratory site and program requirements requirements. The 817 and 818 facilities, originally designed as construction sheds, were built in 1948 and had projected lives of 10 to 15 years. The lives have now been extended by more than a factor of two. These buildings will require extensive structural, mechanical and electrical rehabilitation work if left standing, and will require additional replacement insulation if energy usage levels are to be met.

There are recurring multiple roof leaks which periodically cause damage to work in progress, paperwork, equipment and the building walls. Runoff rivers from heavy rains flow under the buildings, undermining the foundations. The outside walls are heat sieves. Expensive electronic equipment and computers are housed in sprinklered, wooden-framed structures. Facility utilization is severely hampered by these conditions. The present ramshackle housing depresses the morale of employees and makes recruiting more difficult, an important factor in view of the tight electronic employment market.

The proposed building will accommodate a total of 111 persons. This includes all of the Electronics Division permanent and temporary personnel presently housed in Buildings 817 and 818 plus the Applied Mathematics Division, Engineering Division and Supply Division personnel who work directly with EL. Over 34,000 square feet of existing substandard space will be demolished. The operating efficiency of the relocated Electronics personnel will be enhanced because of the new building's improved configuration and because of the closer proximity to program division clients and Applied Mathematics Division counterparts.

The net usable area in the proposed building of 36,800 square feet compares with an existing 31,500 net square feet in the existing space. The difference is largely accounted for by the need to alleviate severe overcrowding in a few of the existing work areas, particularly those now occupied by the Applied Mathematics Division personnel.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Electronics facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 83-E-309

10. Details of Cost Estimate

	Item Cost	Total Cost
a. Engineering design and inspection @ 12% of construction costs, item b.	$	$ 750
b. Construction costs.....		6,300
(1) Site work.....	400	
(2) Buildings - 57,000 sq. ft. at $97.89/sq. ft.	5,580	
(3) Utilities.....	320	
c. Demolition and Removal of Debris.....		185
d. Relocation.....		135
(1) Staff and equipment.....	85	
(2) Microwave antenna (includes setup and power).....	50	
Subtotal.....		7,370
e. Contingency @ 15% of above costs.....		1,130
Total.....		$ 8,500

*Cost estimate based on completed conceptual design report.

11. Method of Performance

Design and inspection will be performed under a negotiated architect/engineer contract. Construction and procurement will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

a. Total Project Costs:	Prior Years	FY 1983	FY 1984	FY 1985	FY 1986	Total
(1) Total facility costs:						
(a) Construction line item.....	$ 0	$ 240	$ 1,600	$ 5,150	$ 1,510	$ 8,500
(b) CP&D.....	0	0	0	0	0	0
(c) Expense funded equipment.....	0	0	0	0	0	0
(d) Inventories.....	0	0	0	0	0	0
Total facility costs.....	0	240	1,600	5,150	1,510	8,500
(2) Other project costs:						
(a) R&D necessary to complete construction	0	0	0	0	0	0
(b) Other project related costs.....	50	0	0	0	0	50
Total other project funding.....	50	0	0	0	0	50
Total Project Funding (items 1 & 2).....	$ 50	$ 240	$ 1,600	$ 5,150	$ 1,510	$ 8,550

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Electronics facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 83-E-309

12. Funding Schedule of Project Funding and Other Related Funding Requirements (continued)

b. Other related annual costs (Estimated life of project: 25 years)	Existing	Proposed	Change
(1) Facility operating costs	174*	243	69
(2) Programmatic operating expenses directly related to the facility	None	None	None
(3) Capital equipment not related to construction but related to the programmatic effort in the facility	124	124	None
(4) GPP or other construction related to programmatic effort in the facility.	75	19	-56
(5) Other costs	None	None	None
Total other related annual funding requirements	373	386	13

*Only minimal maintenance is being performed on existing facilities due to severity of deteriorated condition.

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding:
   1. Total Facility:
      (a) Construction line item - No narrative required.
      (b) PE&D - No narrative required.
      (c) Expense funded equipment - None.
      (d) Inventories - Existing inventories will be transferred from present facilities.
   2. Other project funding:
      (a) R&D necessary to complete construction - None
      (b) Other project related funding - Cost of conceptual design is given.

b. Total related funding requirements: The costs tabulated here are listed in 1983 dollars.
   1. Facility operating costs are a summation of the following cost factors:

Cost Component	Existing	New	Change
Maintenance	33*	139	106
Utilities	56	50	(-6)
Custodial	29	48	19
Major Repair	56	6	(-50)
Total	174	243	69

*Only minimal maintenance is being performed on existing facilities due to severity of deteriorated condition.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Electronics facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 83-E-309

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

2. EL serves many programmatic functions on site, but is not a direct programmatic effort; therefore, this item is recorded as none.
3. Capital equipment is the EL annual equipment budget and will remain constant.
4. GPP or other construction effort will be extensive for the continued use of the existing facilities. The buildings have exceeded their useful life and would have to be substantially rebuilt. The proposed facility expense would reflect roof replacement and major mechanical equipment toward the end of the 25-year estimated life.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

3. Date A-E work initiated: 2nd Qtr. FY 1983

3a. Date physical construction starts: 1st Qtr. FY 1983

4. Date construction ends: 1st Qtr. FY 1986

5. Previous cost estimate: None

6. Current cost estimate: $12,000
Less amount of PE&D: 0
Net Cost Estimate: $12,000
Date: June 1981

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1983	$ 1,300	$ 1,300	$ 1,300	$ 260
1984	10,700	7,500	7,500	2,800
1985	0	3,200	3,200	7,500
1986	0	0	0	1,440

8. Brief Physical Description of Project

This project provides for the installation of a new boiler at the Central Steam Facility, installation of approximately 13,600 ft. of underground steam and condensate piping to serve 22 buildings and the installation of one (1) new water supply well, one million gallon storage tank, other modifications at the Water Treatment Plant Facility and construction of a new recharge basin.

1. The proposed new boiler will have a rated capacity of about 125,000 lbs. per hour at 125 psig., be equipped with an economizer, soot blowers, forced draft fan with electric and steam turbine drives, feed water regulator, steam atomizing high efficiency and clean firing dual fuel burner(s) for burning 100% Alternate Liquid Fuel (ALF), virgin No. 6 fuel oil, various combinations consisting of ALF and virgin fuel oil and coal derived fuels, low excess air firing combustion controls-safety devices and alarms, themix "Corten" stack, etc. The boiler will be connected to associated support systems, both new and modified, consisting of: combustion air, fuel oil, feed water and dearation chemical treatment, steam, electrical, compressed air, drainage, etc.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

8. Brief Physical Description of the Project (continued)

Also included are the required building modifications to the Central Steam Facility for accommodating the new boiler configuration and auxiliary equipment arrangement. These building alterations relate essentially to reinforcing the structural steel members, raising a section of the roof line and the removal and replacement of the building sidewall to facilitate rigging in the new boiler.

2. Underground Steam Main Extension

The proposed steam main extension will provide new heating services for 22 buildings located in the central eastern, and southern sectors of the Laboratory site. It will also result in the retirement of 15 independent and inefficient heating plants and conserve a total of approximately 46,000 gallons of fuel each year. Presently, these 15 units use approximately 165,000 gallons of fuel oil each year consisting of propane, residual and distillate oils. Transferring the heating load to the more efficient Central Steam Plant will result in the overall saving of fuel oil.

All of the steam and condensate lines to be installed will be in a conduit system with both lines insulated to reduce BTU losses. The total designed steam requirement for this project is well within the nominal capacity of the existing Central Steam Facility.

3. Water System Improvements

The expansion of the present Water Treatment Plant Facilities and the installation of one new water supply well is required to meet the water supply requirements of the Laboratory. Expansion work includes a new retention tank, monovalve filter, one million gallon elevated storage tank, interconnecting distribution piping and monitoring/control instrumentation.

Expansion of the plant will also provide bypass piping and modifications to the facilities main flow distribution piping system. The construction of new dual infiltration basins for recharging water and the reorientation and extension of existing drainage piping to a new more distant site with satisfactory permeable ground strata are also included.

9. Purpose, Justification of Need for, and Scope of Project

The purpose of this project is to improve the reliability and efficiency and reduce operating and maintenance costs for the central steam and water utility systems at Brookhaven National Laboratory.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

9. Purpose, Justification of Need for, and Scope of Project (continued)

1. Central Steam Facility

The project will materially improve the operating efficiency and reliability of the Central Steam Facility. The retirement of boiler No. 3, an inefficient 26-year old boiler which has surpassed its standard service life (25 years) and replacing it with an efficiently designed fuel and energy conserving modern boiler will bring the plant into compliance with state and federal particulate emission standards (6 N.Y. CRR Part 277 (c)).

The proposed new boiler will burn a non-critical form of fuel, namely an alternate liquid fuel (ALF) as its source of raw energy input. The ALF used at Brookhaven National Laboratory is formulated by selectively blending feedstocks of recycled or previously used semi-miscible alcohols, mineral spirits, solvents and other combustible liquids to provide a homogeneous fuel of predictable BTU content, viscosity and flash point.

The total raw energy input to the Central Steam Facility is 1,000 billion BTU's annually of liquid fuel to produce steam for the entire Brookhaven National Laboratory site. This proposed project compared to the present mode of operation (using two boilers in lieu of one) will save approximately 105 billion BTU's of raw energy input (750,000 gallons) annually. Another important result benefiting the environment will be the corresponding reduction of boiler stack gas and particulate emissions to the atmosphere.

Under present operating conditions, boiler No. 5 (180,000 lbs/hour) is used for winter operation with boilers No. 3 and/or 4 in peaking or standby condition. With either boiler No. 3 or 4 down for annual service and a wintertime failure of boiler No. 5, the Central Steam Facility would not be able to provide sufficient steam for the various scientific and site facilities.

This boiler replacement will be instrumental in meeting the requirements of Executive Order 12003, the Interim Management Directive, "Fuel and Energy Use Policy for Facilities," and complying with the National Energy Act of 1978.

2. Underground Steam Main Extension

The proposed extension of the underground steam system will replace a 36-year old low-pressure steam distribution system with a new high and low-pressure steam distribution system. The existing low pressure steam distribution piping is essentially a conduit system consisting of magnesia insulated steam and condensate lines supported inside a corrugated metal casing.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

9. Purpose, Justification of Need for, and Scope of Project (continued)

Over the years, fractures have developed in the underground casing that allowed water to enter the conduit system. As the seepage became heated, it dissolved both the insulation and the concrete pipe supports forming a hot alkali solution that then corroded the steel piping over an interval of time. This chemical reaction and subsequent corrosion has occurred at numerous points throughout the system. Not only has it critically impaired the heating system, but steam and condensate leaks have caused the failure of an essential 2400 volt electrical service and seriously jeopardized a 13.8 kV electrical service, fire alarm, and telephone trunk lines. These leaks have resulted in increased make-up water (approximately 6000 gallons per day) at the Central Steam Facility that must be heated and chemically treated. Continuing repairs to this underground steam transport piping and critical ancillary services have proved to be economically and operationally counter-productive toward continuity of scientific and support operations.

The installation of the new high and low-pressure steam mains in the central area of the site, expanding the high-pressure steam distribution system to the warehouse, shops, and maintenance areas, will facilitate:

a. The retirement of 15 individual heating plants burning No. 2 and No. 4 fuel oil and propane which operate at approximately 50 to 60% efficiency. Heating loads will be transferred to the Central Steam Plant which is about 80% efficient and which utilizes alternate liquid fuels that are classified as non-critical or preferred fuels.

b. The conservation of about 46,000 gallons of fuel each year.

c. Increased reliability of heat within the buildings added to the Central Steam System by this project.

d. Compliance with BNL's commitment to minimize air or water pollution and to meet requirements of the Federal Occupational Safety and Health Act, as well as those of the Environmental Protection Agency.

e. Improved steam generation performance as the 15 independently fired heating plants are unattended. The Central Steam Facility is continuously manned and is fully instrumented for pudent monitoring and control of boiler-burner operations.

f. The elimination of hot alkali solution from forming within the 36-year old steam and condensate system and leaking into the soil.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

9. Purpose, Justification of Need for, and Scope of Project (continued)

3. Water System Improvements

In 1977, Brookhaven National Laboratory commissioned Holzmacher, McLendon and Murrell, P.C., to prepare a master plan for the site water system for the next ten years. The master plan included recommendations for the domestic water, cooling water and fire protection needs of the Laboratory complex. Camp, Dresser and McKee was commissioned in 1978 to perform an indepth engineering survey and evaluation fo the Water Treatment Plant Facilities and to develop a master plan based on recommendations for improvement and expansion of the Laboratory water system to meet immediate and future demands in a reliable and cost-effective manner as follows:

a. Additional Well Supply during the summer, peak demand on the domestic water system exceeds the combined pumping capacity of the present well system. The seriousness of this situation has been thoroughly considered and has resulted in the recommendation that an additional well be installed, as soon as possible, to meet these rising water demands.

b. A secondary condition that must be factored into this water supply matrix is the increasing possibility of mechanical and/or electrical failure of existing well pumping equipment due to age and maximum usage. Reinforcement of the well pumpage system with a new well would provide backup against this.

b. Retention Tank

A complete loss of water treatment polant capacity will occur if the present retention tank is removed from online service for maintenance or equipment failure. The analysis of the retention tank design parameters clearly showed that at high water flow rates (4,000 gpm) into the plant, the tank is grossly underdesigned, thus precluding effective treatment. Even at medium or average flows, the tank is several times smaller than required. Both outside engineering firms have confirmed this conclusion.

c. Monovalve Filter

The monovalve sand filters are not adequate to effectively treat peak flows through the plant and an additional 2,500 gpm filter will be added and put in parallel with the other filters. Once constructed, the new filter will provide greater flexibility in day-to-day plant operations by reducing the hydraulic overlead on the older filters, improving process treatment and plant performance during the peak demands which are increasing in frequency and duration each year. It will also provide necessary backup for the other filters during repairs, malfunctions and maintenance, while providing some potential for increased capacity.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

9. Purpose, Justification of Need for, and Scope of Project (continued)

3. Water System Improvements (continued)

d. Storage Tank

The required fire flow for an emergency situation is 4,000 gpm continuously for a four-hour period. BNL does not meet the fire underwriters minimum requirements of supplying the maximum fire flow when required.

Based on the studies that have been done, construction of a one million gallon water tower is required if adequate and reliable protection for fighting a serious fire at the Laboratory is to be reasonably assured.

e. Piping and instrumentation

The addition of a new retention tank and filter will require piping modifications to the plant's raw water system and treated water systems. To assure more flexible and reliable day-to-day and seasonal plant operation, it is planned to provide adequate piping and valves to be able to bypass or isolate each treatment module (e.g., aerator, retention tank, filter, etc.) in the plant treatment system. In this manner, units can be taken out of service for repairs and maintenance without closing down the entire plant as is now required.

To assure that state and federal drinking water standards are met, continuous monitoring and optimization of potable water quality and filter performance can be achieved by the installation of additional instrumentation including: chlorine residual monitors and analyzers, filter effluent turbidimeters, filter loss of head indicators and backwash frequency recorders.

f. Recharge Basins

Camp, Dresser and McKee was also commissioned (1979) to investigate the cause for AGS recharge basin failure and determine what effect their continued heavy loading would have on the underground water table.

At the time of the investigation, the basins were overflowing due to iron plugging of the basin's surface strata, causing severe flooding on the east side of the site. Also, their continued heavy use, over a twenty-year period, has deteriorated and essentially exhausted the percolating capability of the basin's soil formation.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

9. Purpose, Justification of Need for, and Scope of Project (continued)

f. Recharge Basins (continued)

In addition, the heavy loading of the recharge basins has increased the groundwater table in the area. Evidence now exists that a groundwater mound has formed a gradient between the recharged water and the normal underground water sources for the potable wells. These conditions could lead to infiltration, and should be avoided since they could result in water quality degradation and contravene accepted standards of good water management practices.

As a short-term solution to the basin's iron plugging problem, they have been rejuvenated by removing the iron impregnated soil from the surfaces of the basin sides and bottoms. This has eliminated the overflow problem temporarily by improved recharging. This work has been completed by BNL, but is considered only as an interim short-term solution.

As a first step toward the long-term solution of eliminating basin flooding and potential infiltration of present and future well fields, new recharge basins will be constructed away from potable water supply wells and down-gradient in the aquifer. The basins will also be made larger to decrease the area of influence of the recharge.

10. Details of Cost Estimate

		Item Cost	Total Cost
a.	Architect-Engineer, design ad inspection at approximately 12% of Construction Costs		$ 1,100
b.	Construction Costs		9,300
	Central Steam Facility	$ 2,700	
	(1) General construction	$ 457	
	(2) Electrical work	244	
	(3) Mechanical work	563	
	(4) Boiler procurement (incl. accessories)	1,218	
	(5) Boiler erection	218	
	Underground Steam Extension	$ 2,030	
	(1) Central site area	$ 544	
	(2) Warehouse area	929	
	(3) Machine Shop B, Animal Quarantine and Electrical/Mech. Maintenance bldgs.	557	

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

10. Details of Cost Estimate (continued)

	Item Cost	Total Cost
Water System Improvements	4,570	
(1) One domestic water system supply well	500	
(2) Water Treatment Plant Expansion	1,070	
(3) One million gallon elevated storage tank	2,000	
(4) Recharge basins relocation	1,000	
c. Contingency at approximately 15% of above costs		$ 1,600
Total Costs		$12,000

The above contingency of $1,600,000 includes $200,000 for engineering. The additional engineering is essential because of the various design intangibles normally associated with modifying underground utilities and the planned rehabilitation work. Rehabilitation at the Water Treatment Facility includes interfacing new and improved system designs with older existing controls, instrumentation, equipment, etc. Planned physical plant modification at the Central Steam Facility includes integrating the new boiler with existing equipment, fuel train and burner management systems. Past experience at Brookhaven National Laboratory indicates the strong necessity for additional engineering in this type of construction project. This project will not have a significant impact on inflation or increased costs to the private sector.

11. Method of Performance

Design and inspection will be performed under two (2) negotiated architect-engineer lump-sum contracts. Due to the very specialized nature of these utility improvements, single A/E firms do not usually specialize in both steam plant and water utility design work. Therefore, it is contemplated that one A/E firm be selected for the steam plant modification and underground steam main extensions and a second A/E firm be selected for the design work for the water system improvements. Construction and procurement will be accomplished by fixed-price contracts and purchase orders awarded on the basis of competitive bidding.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1983	FY 1984	FY 1985	FY 1986	Total
a. Total project costs:						
1. Total facility costs:						
(a) Construction line item	$ 0	$ 260	$ 2,800	$ 7,500	$ 1,440	$12,000
(b) PE&D	0	0	0	0	0	0
(c) Expense funded equipment	0	0	0	0	0	0
(d) Inventories	0	0	0	0	0	0
Total facility costs	$ 0	$ 260	$ 2,800	$ 7,500	$ 1,440	$12,000
2. Other project costs						
(a) R&D necessary to complete construction	$ 0	$ 0	$ 0	$ 0	$ 0	$ 0
(b) Other project related costs	200	0	0	0	0	200
Total other project costs	200	0	0	0	0	200
Total project costs	$ 200	$ 260	$ 2,800	$ 7,500	$ 1,440	$12,200

b. Other related annual costs (estimated life of project: 30 years)	
1. Facility operating costs	$ - 738
2. Programmatic operating expenses directly related to the facility	0
3. Capital equipment not related to construction but related to the programmatic effort of this facility	0
4. GPP or other construction related to the programmatic effort in the facility	0
5. Other costs	0
Total other related annual costs	$ - 738

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Utility replacements and upgrade
Brookhaven National Laboratory, Upton, N.Y.

2. Project No.: 83-E-310

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
   1. Total facility
      (a) Construction line item - See Item 10.
      (b) PE&D - Not applicable.
      (c) Expense funded equipment - Not applicable.
      (d) Inventories - Not applicable.
   2. Other project funding
      (a) R&D - Not applicable.
      (b) Other project related costs - Conceptual design costs total $200,000.

b. Total related funding requirements
   1. After completing these improvements, the annual operating cost for these utilities is estimated as follows:

(a) Maintenance and Operations	$1,115,000
(b) Energy (utilities)	3,695,000
Total Operating Costs	$4,810,000

   2. However, if these utility improvements are not funded, the existing utility system will have a total annual operating cost as follows:

(a) Maintenance and Operations	$1,221,000
(b) Energy (utilities)	4,327,000
Total Operating Costs	$5,548,000

      Therefore, it is estimated that there would be annual savings of $738,000 for these proposed utility improvements.
   3. Programmatic Operating Expense Directly Related to the Facility: Not applicable.
   4. Capital Equipment not Related to Construction but Related to the Programmatic Effort in the Facility: Not applicable.
   5. GPP or other Construction Related to Programmatic Effort: Not applicable.
   6. Other Costs: Not applicable.

DEPARTMENT OF ENERGY
1985 CONGRESSIONAL BUDGET REQUEST
CONSTRUCTION PROJECT DATA SHEETS
ENERGY SUPPLY RESEARCH AND DEVELOPMENT - PLANT AND CAPITAL EQUIPMENT
MULTIPROGRAM GENERAL PURPOSE FACILITIES
(Tabular dollars in thousands. Narrative material in whole dollars.)

1. Title and location of project: Security facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 82-E-302

3. Date A-E work initiated: 1st Qtr. FY 1982

3a. Date physical construction starts: 1st Qtr. FY 1983

4. Date construction ends: 4th Qtr. FY 1985

5. Previous cost estimate: None

6. Current cost estimate: $ 8,100
Less amount of PE&D: 0
Net Cost Estimate: $ 8,100
Date: May 1980

7. Financial Schedule:

Fiscal Year	Authorizations	Appropriations	Obligations	Costs
1982	$ 1,500	$ 1,500	$ 1,500	$ 25
1983	3,200	3,200	3,200	1,485
1984	3,400	2,300	2,300	2,000
1985	0	1,100	1,100	4,590

8. Brief Physical Description of Project

This project provides for new facilities for the Security Division (SEC), and a new site-wide Alarm Communication and Appraisal System (ACAS). This facility will house SEC personnel for a three shift operation 24 hours per day seven days per week. All personnel use building facilities for lockers, toilets, lunch, report writing and personnel supervision and administration. Personnel using the building on a full-time or part-time basis will total approximately 120 personnel. Parking facilities for approximately 70 vehicles will be provided.

The building is to meet agency minimum standards and provide a functional, energy efficient facility for SEC space; hardened primary command center for ACAS; secure weapons storage; offices, locker areas, assembly/briefing area, and training areas for personnel with a special purpose training area for riot control/physical security response training; weapons firing range; and exercise area; required storage for records, uniforms, and security equipment; and a suitable lockshop.

The structure will consist of a single story building with lower level hardened central station and mid-level multipurpose training space. The gross area of the building will be approximately 24,000 square feet. The building is planned to have a steel frame with masonry curtain wall. Exterior glazing will be limited and earth berming will be used for thermal efficiency.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Security facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 82-E-302

8. Brief Physical Description of the Project (continued)

Partitions will be systems compatible with use, flexibility and life cycle cost. Final design procedures will include an update on construction life-cycle costs and energy efficient materials to assure maximum overall efficiency.

The Alarm System will consist of:

a. A dedicated security transmission cable loop around the Inner Circle Drive connected to Buildings 200, 202, 205, 208 and 212; a connection to Building 395 for the auxiliary command center; and a secondary loop to Building 331. This cable will be direct burial or carried with existing steam or utility lines as determined by final engineering and cost analysis. The cable will have a shielded line with coaxial video signal lines to carry high-speed data and video signals.

b. The Alarm Communications System with signal transponders in all buildings that have sensors; data processing monitors and graphic displays at primary and secondary command stations; LED displays and high-speed printers to record time, data sensor, and alarm or tamper; and a serially addressed test key system. Approximately 600 sensors are to be installed by 1981. The new system must connect to these 600 sensors and will have sufficient capacity for 400 additional sensors. The system will be computer compatible; however, no computer installation is anticipated at this time. Digitally driven random access microfilm projectors with facility maps and response directions will be provided in primary and secondary command centers.

c. The Video Alarm Appraisal and Surveillance System will provide pan-tilt, low-light television cameras with zoom lenses at this building and at Buildings 212, 316, 331 and 350 to cover perimeter alarm zones; and material access control identification and surveillance cameras both tied to and controlled from the primary and secondary command centers.

9. Purpose, Justification of Need For, and Scope of Project

The Security Division's functions are related either directly or indirectly to three basic responsibilities: (a) protection of Laboratory personnel from injury or harassment, (b) protection of Laboratory property from theft, misappropriation or deliberate damage, and (c) protection of Laboratory classified information from loss or compromise. Security's present housing is in an old, energy inefficient, "temporary" Quonset hut which provides an inadequate amount, nature and quality of space. There is inadequate storage area for armament as well as special equipment that is needed to meet agency requirements for protection of special nuclear materials. An expanded armory with improved physical security, additional storage and maintenance space will be provided.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Security facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 82-E-302

9. Purpose, Justification of Need For, and Scope of Project (continued)

Security's vehicle fleet is parked in an open area. This facility will include a protected parking area.

The Central Alarm Station, which monitors critical areas, is also vulnerable. The room lacks adequate floor space for the future expansion of alarm coverage, communications equipment, and other items which are planned for a more efficient viable alarm station.

The need for a dedicated cable system is justified on the basis that the present telephone lines are: (a) inadequate for high-speed data video signal transmission; (b) cannot be expanded to meet the need to monitor approximately 600 sensor points; (c) susceptible to false alarm and failure due to lightning and electromagnetic interference; and (d) vulnerable to defeat by unsophisticated substitution components at unprotected telephone junction boxes.

The need for a multiplex digital alarm control system is justified on the basis of the inadequacy of the present 75-zone system for providing information for timely response to over 600 sensors presently being installed under the Safeguard and Security Improvement Program, and the agency requirement for a duplicate alarm monitoring capability at a primary and a secondary security command station.

The cable, alarm processing, and video system are mutually supportive and are needed as an integrated security system.

10. Details of Cost Estimate

	Item Cost	Total Cost
a. Engineering design and inspection @ 12% of construction costs, item b.	$	$ 399
b. Construction costs.....		3,324
(1) Site work.....	204	
(2) Buildings - 24,000 sq. ft. at $117/sq. ft.	2,809	
(3) Utilities.....	311	
c. Equipment.....		3,202
(1) Security Equipment.....	129	
(2) Alarm communication and appraisal system.....	3,073	
d. Demolition of vacated structures and relocation costs.....		128
Subtotal.....		7,053
e. Contingency @ 15% of above costs.....		1,047
Total.....		$ 8,100

*Cost estimate based on a completed conceptual design.

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Security facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 82-E-302

11. Method of Performance

Design and inspection will be performed under a negotiated architect/engineer contract. Construction and procurement will be accomplished by fixed-price contracts awarded on the basis of competitive bidding, with the exception of the classified work of the ACAS which will be accomplished under a cost-plus-fixed fee (CPFF) contract.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1982	FY 1983	FY 1984	FY 1985	Total
a. Total project costs:						
1. Total facility costs:						
(a) Construction line item	$ 0	$ 25	$ 1,485	$ 2,000	$ 4,590	$ 8,100
(b) PE&D	0	0	0	0	0	0
(c) Expense funded equipment	0	0	0	0	0	0
(d) Inventories	0	0	0	0	0	0
Total facility costs	0	25	1,485	2,000	4,590	8,100
2. Other project costs:						
(a) R&D necessary to complete construction	25	0	0	0	0	25
(b) Other project related costs	0	0	0	0	0	0
Total other project costs	25	0	0	0	0	50
Total project costs (items 1 & 2)	$ 25	$ 25	$ 1,485	$ 2,000	$ 4,590	$ 8,125

b. Other related annual costs (estimated life of project: 25 years)	
1. Facility operating costs	$ 0
2. Programmatic operating expenses directly related to the facility	0
3. Capital equipment not related to construction but related to the programmatic effort in the facility	0
4. GPP or other construction related to programmatic effort in the facility	0
5. Other costs	0
Total other related annual costs	$ 0

CONSTRUCTION PROJECT DATA SHEETS

1. Title and location of project: Security facility, Argonne National Laboratory, Argonne, IL

2. Project No.: 82-E-302

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
   1. Total facility
      (a) Construction Line Item: No narrative required.
      (b) PE&D: No narrative required.
      (c) Expense Funded Equipment: None
      (d) Inventories: Existing inventories will be transferred from present facilities.

   2. Other Project Funding
      (a) R&D Necessary to Complete Construction: Approximately $25,000 was spent in developing the conceptual design.
      (b) Other Project Related Funding: None

b. Total related funding requirements: Facility operating costs, shown as $0, reflect the fact that no additional personnel will be hired to occupy the building and that construction of the building will result in a net savings in operating costs due to the energy conserving construction which will be utilized.